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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	SEP 09	CA/CAplus records now contain indexing from 1907 to the present
NEWS 4	DEC 08	INPADOC: Legal Status data reloaded
NEWS 5	SEP 29	DISSABS now available on STN
NEWS 6	OCT 10	PCTFULL: Two new display fields added
NEWS 7	OCT 21	BIOSIS file reloaded and enhanced
NEWS 8	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 9	NOV 24	MSDS-CCOHS file reloaded
NEWS 10	DEC 08	CABA reloaded with left truncation
NEWS 11	DEC 08	IMS file names changed
NEWS 12	DEC 09	Experimental property data collected by CAS now available in REGISTRY
NEWS 13	DEC 09	STN Entry Date available for display in REGISTRY and CA/CAplus
NEWS 14	DEC 17	DGENE: Two new display fields added
NEWS 15	DEC 18	BIOTECHNO no longer updated
NEWS 16	DEC 19	CROPU no longer updated; subscriber discount no longer available
NEWS 17	DEC 22	Additional INPI reactions and pre-1907 documents added to CAS databases
NEWS 18	DEC 22	IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19	DEC 22	ABI-INFORM now available on STN
NEWS 20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS 21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS 22	FEB 05	German (DE) application and patent publication number format changes

NEWS EXPRESS	DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:17:47 ON 01 MAR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:17:53 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9
DICTIONARY FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

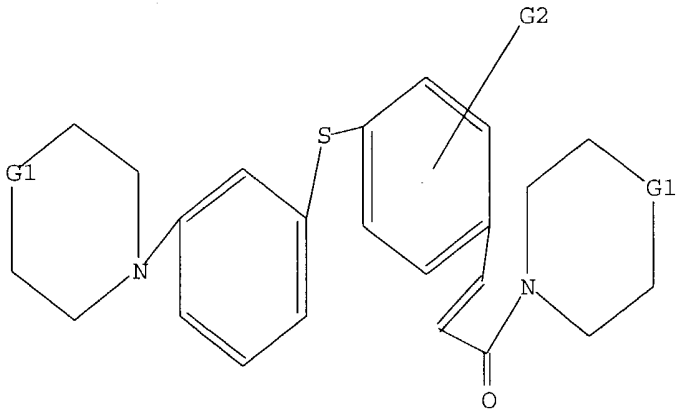
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\09541795.11

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,O,S,N,NH,CH2,CH

G2 CF3,X

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 16:18:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 37 TO ITERATE

100.0% PROCESSED 37 ITERATIONS 28 ANSWERS
SEARCH TIME: 00.00.01

L2 28 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 16:18:30 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 1 Mar 2004 VOL 140 ISS 10
FILE LAST UPDATED: 29 Feb 2004 (20040229/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L3            2 L2

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L3   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2000:725609  CAPLUS
DN   133:296281
TI   Preparation of 2- or 4-(phenylthio)cinnamides as cell adhesion-inhibiting
     antiinflammatory and immune-suppressive compounds
IN   Link, James; Liu, Gang; Pei, Zhonghua; Von Geldern, Thomas W.; Winn,
     Martin; Xin, Zhili; Wang, Sheldon; Boyd, Steven A.; Zhu, Gui-Dong;
     Freeman, Jennifer C.; Gunawardana, Indrani W.; Staeger, Michael A.; Jae,
     Hwan-soo; Lynch, John K.
PA   Abbott Laboratories, USA
SO   PCT Int. Appl., 476 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
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             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
             SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW,
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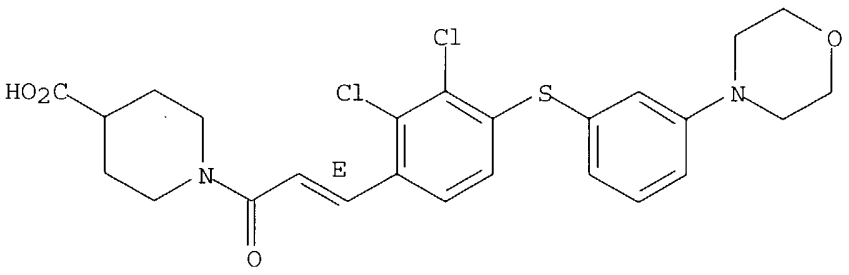
OS MARPAT 133:296281

IT **280752-45-6P 301179-05-5P 301179-08-8P**
301179-10-2P 301179-11-3P 301179-14-6P
301179-21-5P 301179-23-7P 301179-24-8P
301179-25-9P 301179-26-0P 301179-29-3P
301179-30-6P 301179-31-7P 301179-36-2P
301179-37-3P 301179-38-4P 301179-39-5P
301179-40-8P 301179-41-9P 301179-42-0P
301179-43-1P 301179-48-6P 301179-49-7P
301179-59-9P 301179-60-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

RN 280752-45-6 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[2,3-dichloro-4-[[3-(4-morpholinyl)phenyl]thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

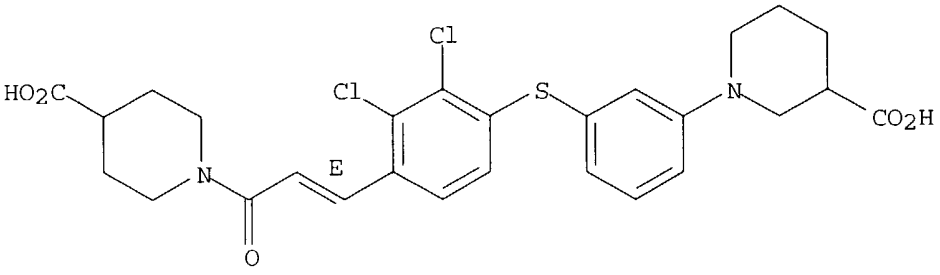
Double bond geometry as shown.



RN 301179-05-5 CAPLUS

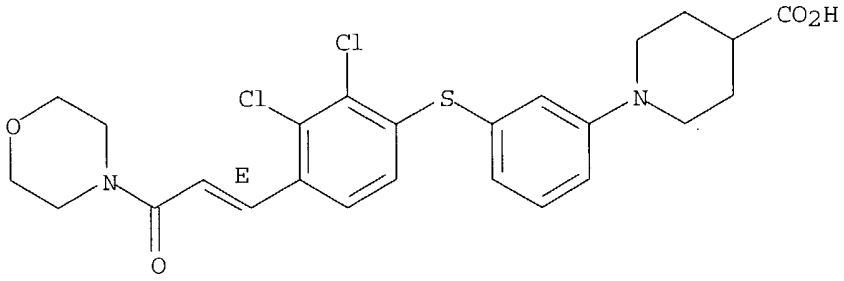
CN 3-Piperidinecarboxylic acid, 1-[3-[[4-[(1E)-3-(4-carboxy-1-piperidinyl)-3-oxo-1-propenyl]-2,3-dichlorophenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



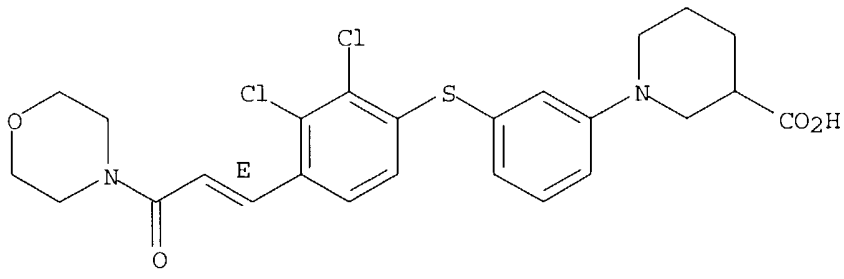
RN 301179-08-8 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-(4-morpholinyl)-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



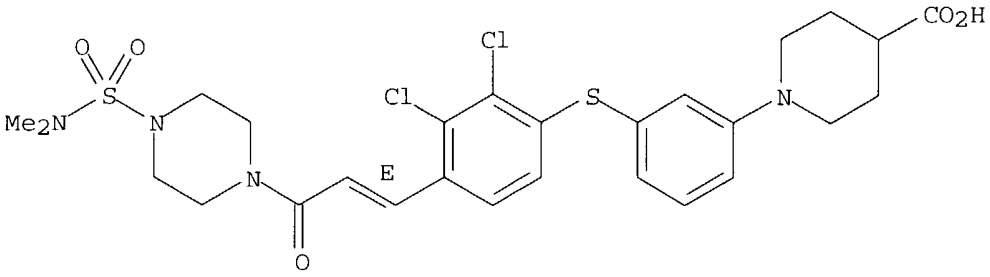
RN 301179-10-2 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-(4-morpholinyl)-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



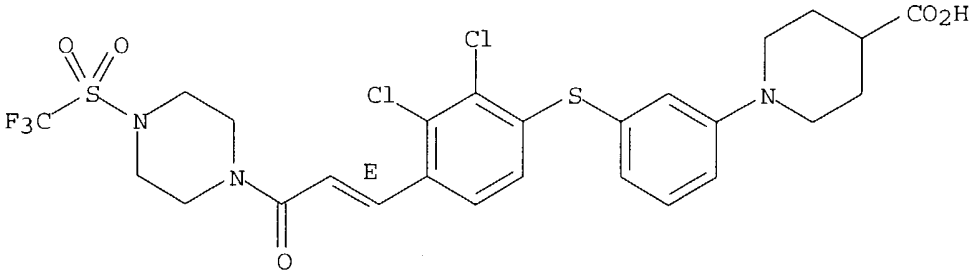
RN 301179-11-3 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-[4-[(dimethylamino)sulfonyl]-1-piperazinyl]-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



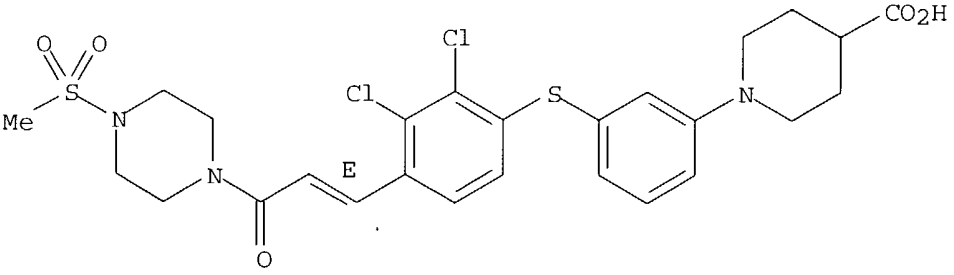
RN 301179-14-6 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-oxo-3-[4-[(trifluoromethyl)sulfonyl]-1-piperazinyl]-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



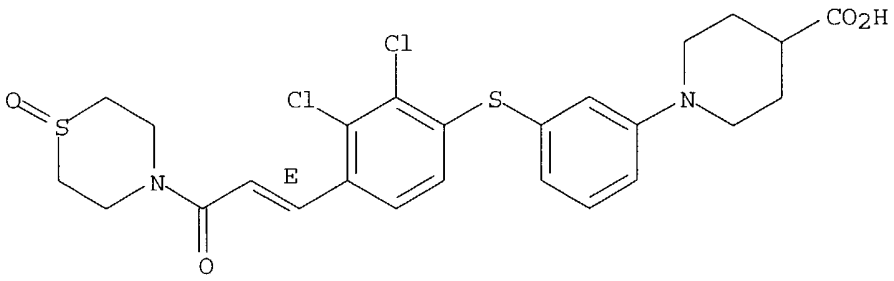
RN 301179-21-5 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-[4-(methylsulfonyl)-1-piperazinyl]-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 301179-23-7 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-(1-oxido-4-thiomorpholinyl)-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

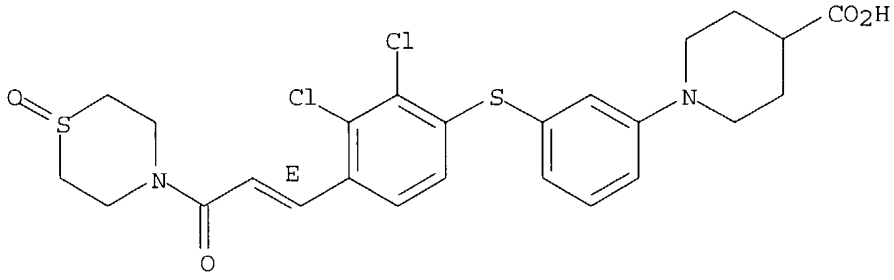


RN 301179-24-8 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-(1-oxido-4-thiomorpholinyl)-3-oxo-1-propenyl]phenyl]thio]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

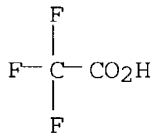
CRN 301179-23-7
CMF C25 H26 Cl2 N2 O4 S2

Double bond geometry as shown.



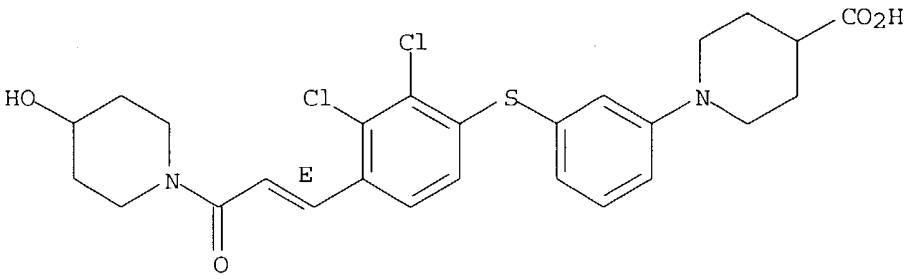
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 301179-25-9 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-(4-hydroxy-1-piperidinyl)-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

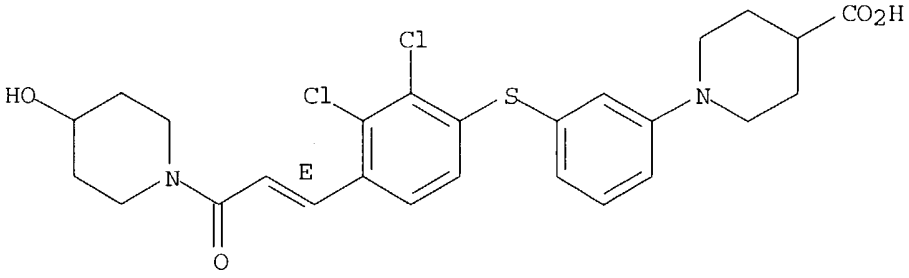


RN 301179-26-0 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-(4-hydroxy-1-piperidinyl)-3-oxo-1-propenyl]phenyl]thio]phenyl]-, trifluoroacetate (4:1) (salt) (9CI) (CA INDEX NAME)

CM 1

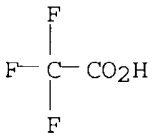
CRN 301179-25-9
CMF C26 H28 Cl2 N2 O4 S

Double bond geometry as shown.



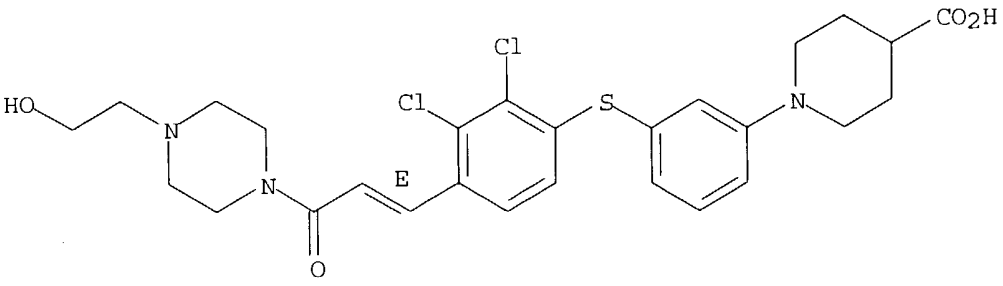
CM 2

CRN 76-05-1
CMF C2 H F3 O2



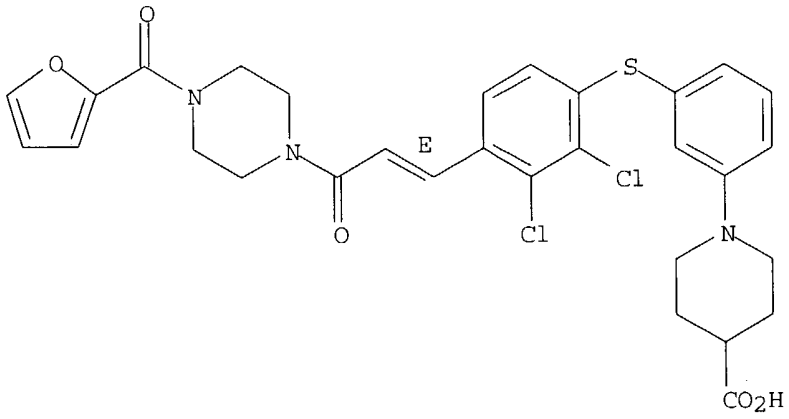
RN 301179-29-3 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-[4-(2-hydroxyethyl)-1-piperazinyl]-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 301179-30-6 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-[4-(2-furanylcarbonyl)-1-piperazinyl]-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

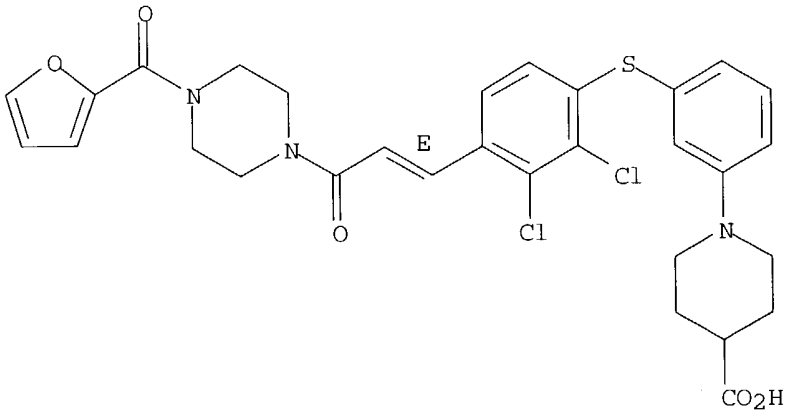


RN 301179-31-7 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-[4-(2-furanylcarbonyl)-1-piperazinyl]-3-oxo-1-propenyl]phenyl]thio]phenyl]-, trifluoroacetate (2:3) (9CI) (CA INDEX NAME)

CM 1

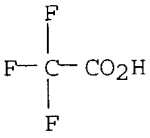
CRN 301179-30-6
CMF C30 H29 Cl2 N3 O5 S

Double bond geometry as shown.



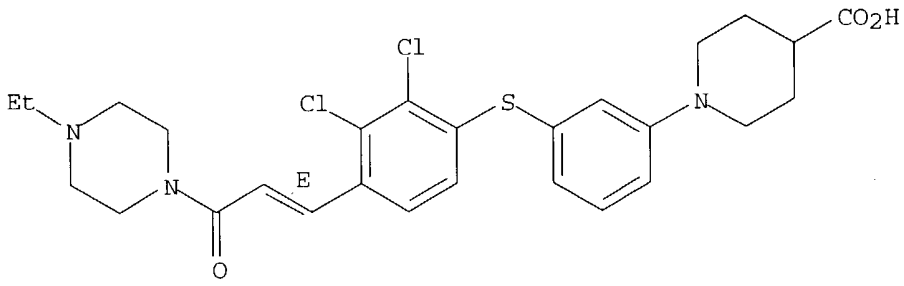
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 301179-36-2 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-(4-ethyl-1-piperazinyl)-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

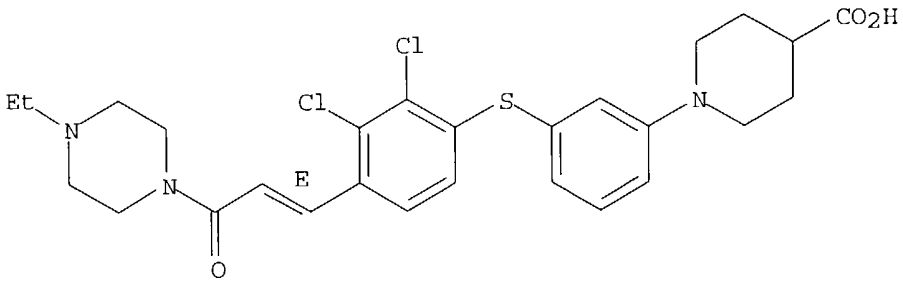


RN 301179-37-3 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-(4-ethyl-1-piperazinyl)-3-oxo-1-propenyl]phenyl]thio]phenyl]-, trifluoroacetate (5:11) (9CI) (CA INDEX NAME)

CM 1

CRN 301179-36-2
CMF C27 H31 Cl2 N3 O3 S

Double bond geometry as shown.



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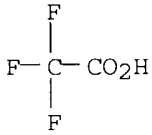
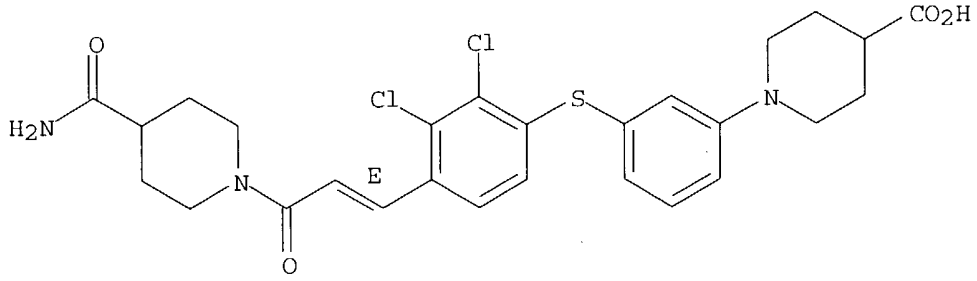
CRN 76-05-1
CMF C2 H F3 O2



RN 301179-38-4 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[4-[(1E)-3-[4-(aminocarbonyl)-1-piperidinyl]-3-oxo-1-propenyl]-2,3-dichlorophenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

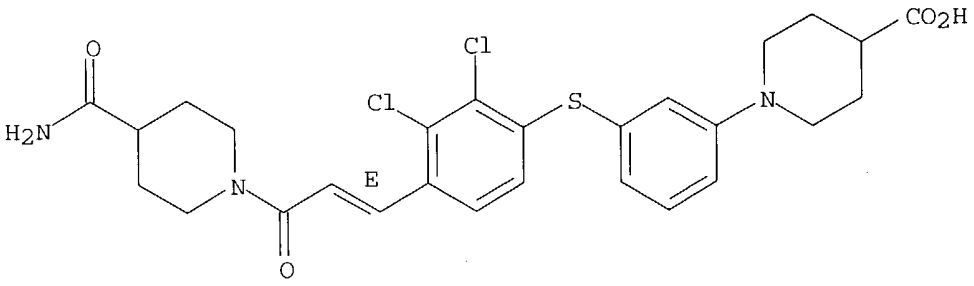


RN 301179-39-5 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[4-[(1E)-3-[4-(aminocarbonyl)-1-piperidinyl]-3-oxo-1-propenyl]-2,3-dichlorophenyl]thio]phenyl]-, trifluoroacetate (5:1) (9CI) (CA INDEX NAME)

CM 1

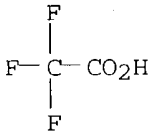
CRN 301179-38-4
CMF C27 H29 Cl2 N3 O4 S

Double bond geometry as shown.



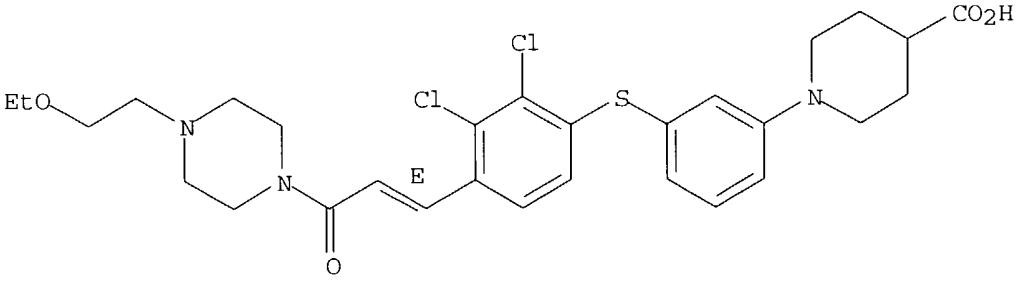
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 301179-40-8 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-[4-(2-ethoxyethyl)-1-piperazinyl]-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

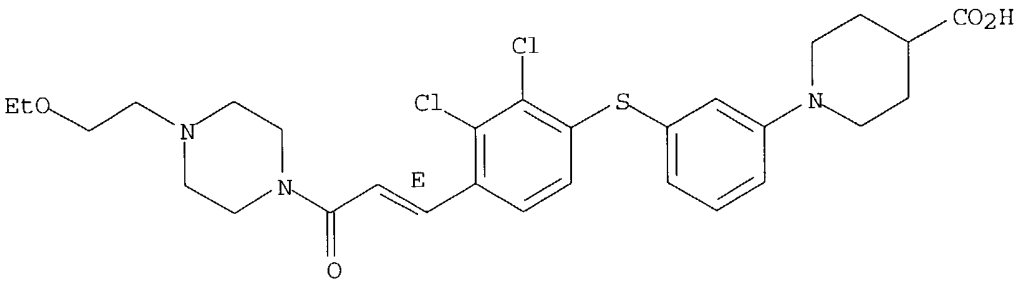


RN 301179-41-9 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-[4-(2-ethoxyethyl)-1-piperazinyl]-3-oxo-1-propenyl]phenyl]thio]phenyl]-, trifluoroacetate (2:5) (9CI) (CA INDEX NAME)

CM 1

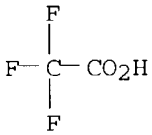
CRN 301179-40-8
CMF C29 H35 Cl2 N3 O4 S

Double bond geometry as shown.



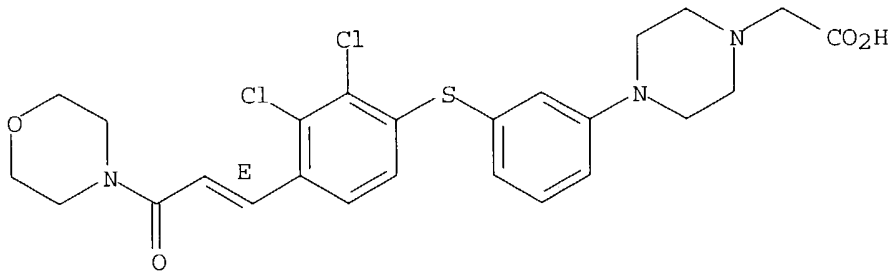
CM 2

CRN 76-05-1
CMF C2 H F3 O2



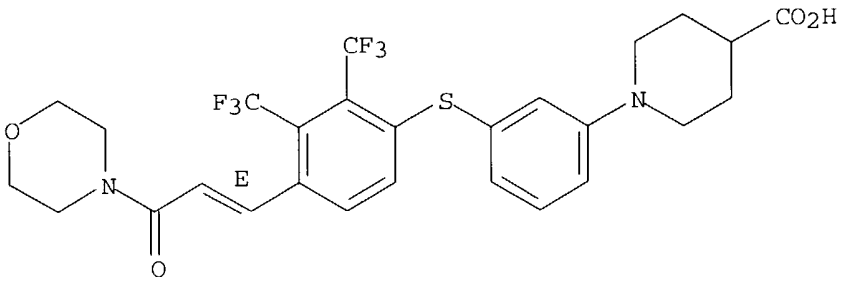
RN 301179-42-0 CAPLUS
CN 1-Piperazineacetic acid, 4-[3-[[2,3-dichloro-4-[(1E)-3-(4-morpholinyl)-3-oxo-1-propenyl]phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



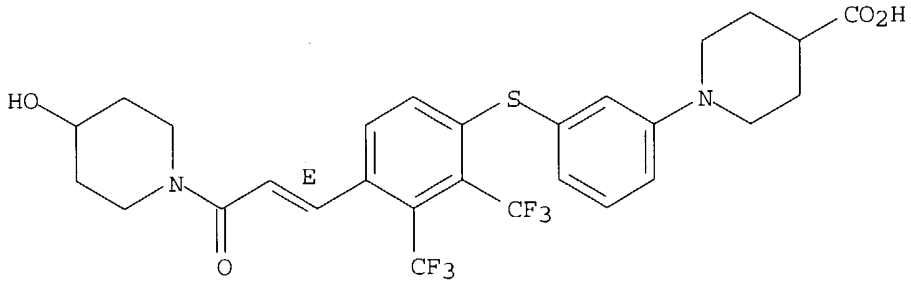
RN 301179-43-1 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[4-[(1E)-3-(4-morpholinyl)-3-oxo-1-propenyl]-2,3-bis(trifluoromethyl)phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 301179-48-6 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[4-[(1E)-3-(4-hydroxy-1-piperidinyl)-3-oxo-1-propenyl]-2,3-bis(trifluoromethyl)phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

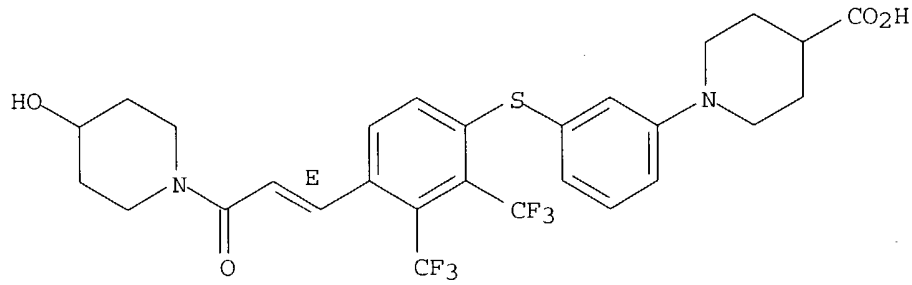


RN 301179-49-7 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[4-[(1E)-3-(4-hydroxy-1-piperidinyl)-3-oxo-1-propenyl]-2,3-bis(trifluoromethyl)phenyl]thio]phenyl]-, trifluoroacetate (20:23) (salt) (9CI) (CA INDEX NAME)

CM 1

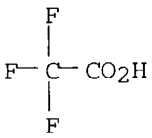
CRN 301179-48-6
CMF C28 H28 F6 N2 O4 S

Double bond geometry as shown.



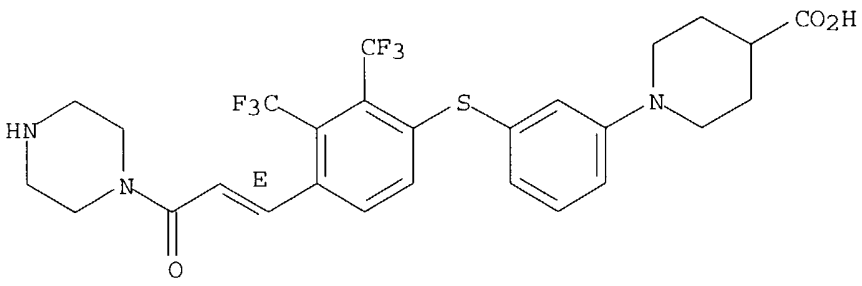
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 301179-59-9 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[4-[(1E)-3-oxo-3-(1-piperazinyl)-1-propenyl]-2,3-bis(trifluoromethyl)phenyl]thio]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

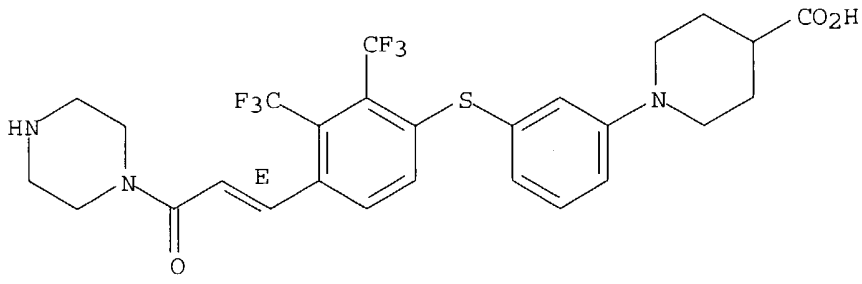


RN 301179-60-2 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[4-[(1E)-3-oxo-3-(1-piperazinyl)-1-propenyl]-2,3-bis(trifluoromethyl)phenyl]thio]phenyl]-, trifluoroacetate (10:33) (9CI) (CA INDEX NAME)

CM 1

CRN 301179-59-9
CMF C27 H27 F6 N3 O3 S

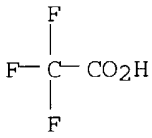
Double bond geometry as shown.



CM 2

CRN 76-05-1

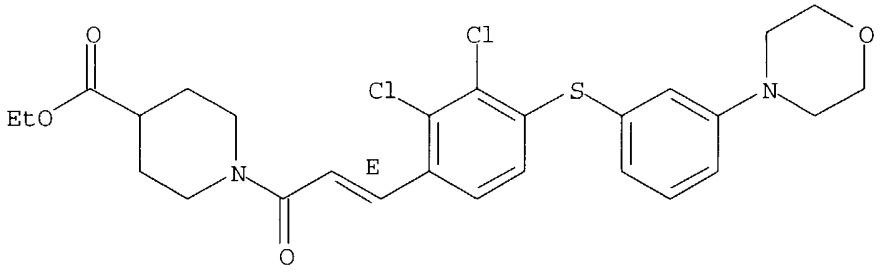
CMF C2 H F3 O2



IT **280753-31-3P 301180-00-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

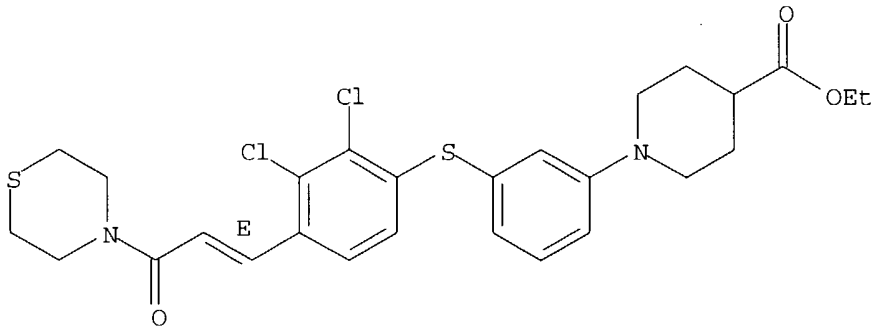
RN 280753-31-3 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[2,3-dichloro-4-[[3-(4-morpholinyl)phenyl]thio]phenyl]-1-oxo-2-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 301180-00-7 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[[2,3-dichloro-4-[(1E)-3-oxo-3-(4-thiomorpholinyl)-1-propenyl]phenyl]thio]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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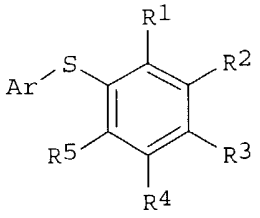

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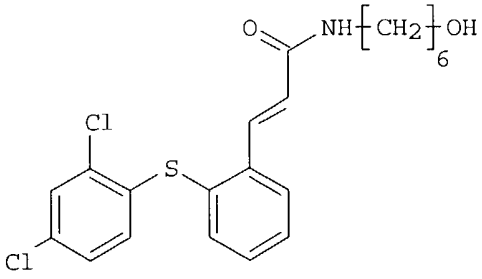

II

AB The title compds. (I) [wherein R1-R5 = independently H, halo, (halo)alkyl, alkoxy, cyano, NO2, CHO, and least one of R1 or R3 is an (un)substituted cis- or trans-cinnamide; Ar = (un)substituted (hetero)aryl] were prepared as cell adhesion inhibitors for the treatment of inflammatory and immune diseases. Examples include syntheses for 443 invention compds. and data for 3 bioassays. For instance, a mixture of 2-[(2,4-dichlorophenyl)thio]benzaldehyde (preparation given), malonic acid, piperidine in anhydrous pyridine was heated at 110°C for 2 h and then treated with aqueous HCl to give trans-2-[(2,4-dichlorophenyl)thio]cinnamic acid (91%). Conversion to the acid chloride followed by amidation with 6-amino-1-hexanol gave (E)-II (90%). In an integrin LFA-1/ICAM-1 biochem. interaction assay, I demonstrated inhibition at 4 μM. In cell-based adhesion assays which measure the ability of test compds. to block adherence of JY-8 cells (a human EBV-transformed B cell line expressing LFA-1 on its surface) to immobilized ICAM-1 or ICAM-3, I exhibited blocking activity at 4 μM and 0.6 μM, resp.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:457022 CAPLUS
DN 133:89514
TI Cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds
IN Link, James; Liu, Gang; Pei, Zhonghua; Von Geldern, Tom; Winn, Martin; Xin, Zhili; Boyd, Steven A.; Jae, Hwan-Soo; Lynch, John K.; Zhu, Gui-Dong; Freeman, Jennifer C.; Gunawardana, Indrani W.; Staeger, Michael A.
PA Abbott Laboratories, USA
SO PCT Int. Appl., 400 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000039081	A2	20000706	WO 1999-US31162	19991229
	WO 2000039081	A3	20010525		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

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NEWS 18	DEC 22	IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19	DEC 22	ABI-INFORM now available on STN
NEWS 20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS 21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS 22	FEB 05	German (DE) application and patent publication number format changes

NEWS EXPRESS	DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
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FILE 'HOME' ENTERED AT 16:17:47 ON 01 MAR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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STRUCTURE FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9
DICTIONARY FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

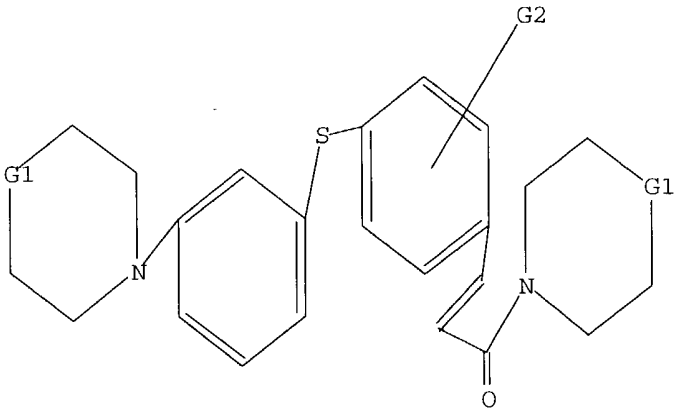
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\09541795.11

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,O,S,N,NH,CH2,CH

G2 CF3,X

Structure attributes must be viewed using STN Express query preparation.

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FULL SEARCH INITIATED 16:18:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      37 TO ITERATE

100.0% PROCESSED       37 ITERATIONS                              28 ANSWERS
SEARCH TIME: 00.00.01

L2            28 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   155.42     155.63

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FILE COVERS 1907 - 1 Mar 2004  VOL 140 ISS 10
FILE LAST UPDATED: 29 Feb 2004  (20040229/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
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=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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DICTIONARY FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\09541795.13

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 16:42:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 441 TO ITERATE

100.0% PROCESSED 441 ITERATIONS 106 ANSWERS
SEARCH TIME: 00.00.01

L2 106 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 16:42:50 ON 01 MAR 2004

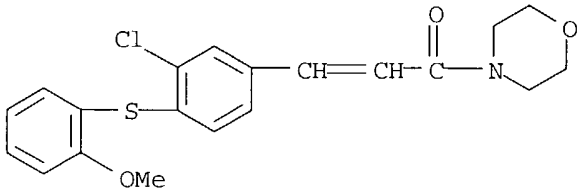
FILE COVERS 1907 - 1 Mar 2004 VOL 140 ISS 10
FILE LAST UPDATED: 29 Feb 2004 (20040229/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

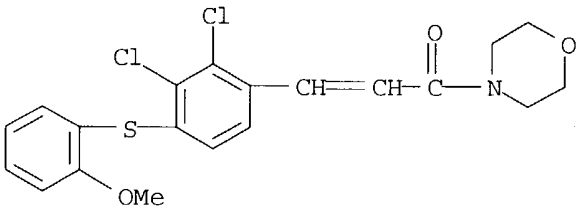
=> s l2
L3 4 L2

=> d l3 fbib hitstr abs total

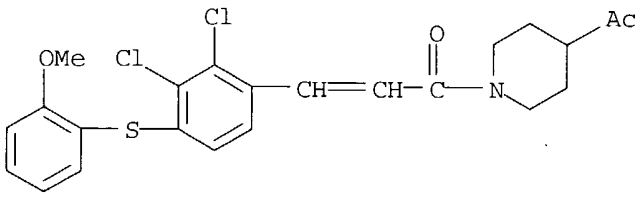
L3 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:235035 CAPLUS
DN 139:285618
TI QSAR Study on Some p-Arylthio Cinnamides as Antagonists of Biochemical ICAM-1/LFA-1 Interaction and ICAM-1/JY-8 Cell Adhesion in Relation to Anti-inflammatory Activity
AU Debnath, Bikash; Samanta, Soma; Roy, Kunal; Jha, Tarun
CS Department of Pharmaceutical Technology, Division of Pharmaceutical and Medicinal Chemistry, Jadavpur University, Kolkata, 700 032, India
SO Bioorganic & Medicinal Chemistry (2003), 11(8), 1615-1619
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
IT **609841-80-7 609841-90-9 609841-91-0**
609841-95-4 609841-96-5 609841-97-6
609842-01-5 609842-02-6 609842-03-7
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR study on arylthio cinnamides as antagonists of biochem. ICAM-1/LFA-1 interaction and ICAM-1/JY-8 cell adhesion)
RN 609841-80-7 CAPLUS
CN Morpholine, 4-[3-[3-chloro-4-[(2-methoxyphenyl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



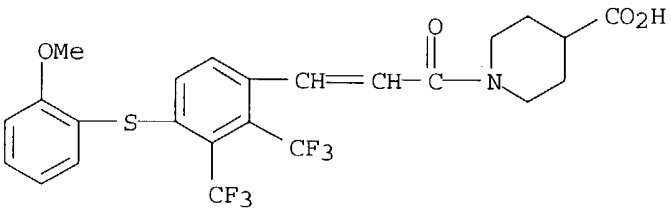
RN 609841-90-9 CAPLUS
CN Morpholine, 4-[3-[2,3-dichloro-4-[(2-methoxyphenyl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



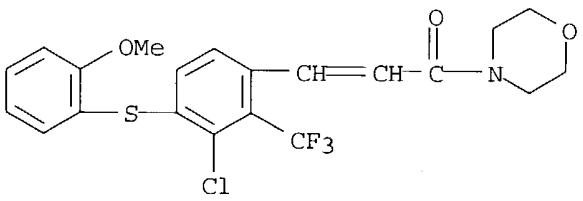
RN 609841-91-0 CAPLUS
CN Piperidine, 4-acetyl-1-[3-[2,3-dichloro-4-[(2-methoxyphenyl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



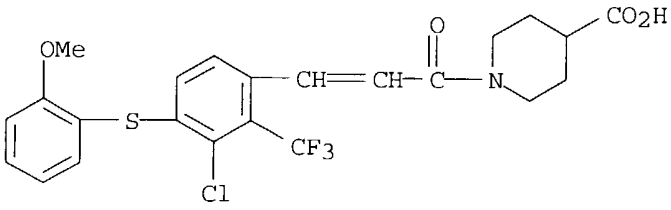
RN 609841-95-4 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[4-[(2-methoxyphenyl)thio]-2,3-bis(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



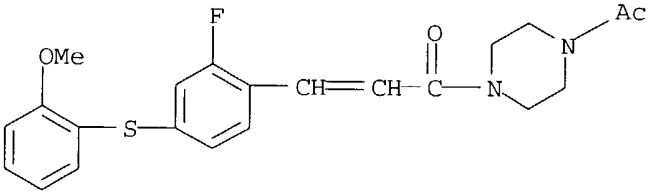
RN 609841-96-5 CAPLUS
CN Morpholine, 4-[3-[3-chloro-4-[(2-methoxyphenyl)thio]-2-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



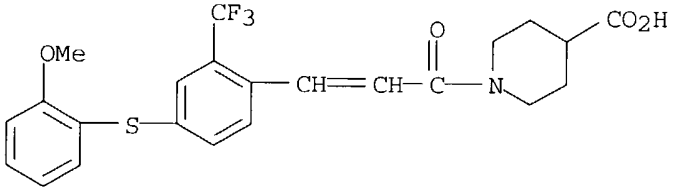
RN 609841-97-6 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[3-chloro-4-[(2-methoxyphenyl)thio]-2-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



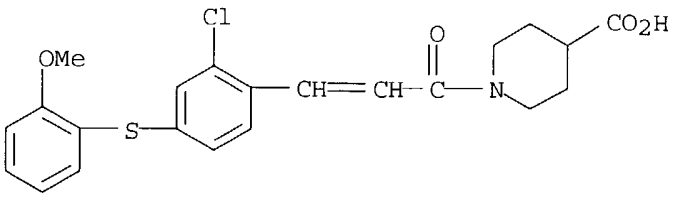
RN 609842-01-5 CAPLUS
CN Piperazine, 1-acetyl-4-[3-[2-fluoro-4-[(2-methoxyphenyl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 609842-02-6 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[4-[(2-methoxyphenyl)thio]-2-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 609842-03-7 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[2-chloro-4-[(2-methoxyphenyl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



AB To find out the chemical and structural features of some p-arylthio cinnamides 1 as antagonists of biochem. ICAM-1/LFA-1 interaction as well as ICAM-1/JY-8 cell adhesion in relation to anti-inflammatory activity, QSAR study was performed. Steric effect on the arylthio ring and lipophilic substitutions at 2,3-positions, especially 2,3-disubstitution with Cl or CF3 or both on cinnamides 1 were conducive to the activity, whereas simultaneous presence of methoxy group at arylthio ring and NCOCH3 group at heterocyclic ring of cinnamides 1 were detrimental to activity in antagonism of biochem. ICAM-1/LFA-1 interaction. When inhibition of ICAM-1/JY-8 cell adhesion was considered, lipophilic substitution on ring B and simultaneous presence of CF3 groups at 2 and 3 positions of the ring B were advantageous to antagonism. This QSAR study showed that B ring has played the most important role for both types of activities.

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:758465 CAPLUS
DN 136:47984
TI Discovery of Novel p-Arylthio Cinnamides as Antagonists of Leukocyte Function-Associated Antigen-1/Intercellular Adhesion Molecule-1 Interaction. 4. Structure-Activity Relationship of Substituents on the Benzene Ring of the Cinnamide
AU Winn, Martin; Reilly, Edward B.; Liu, Gang; Huth, Jeffrey R.; Jae, Hwan-Soo; Freeman, Jennifer; Pei, Zhonghua; Xin, Zhili; Lynch, John; Kester, Jeff; von Geldern, Thomas W.; Leitza, Sandra; DeVries, Peter; Dickinson, Robert; Mussatto, Donna; Okasinski, Gregory F.
CS Metabolic Disease Research Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064-6098, USA
SO Journal of Medicinal Chemistry (2001), 44(25), 4393-4403
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
IT **280749-37-3P 280751-73-7P 280751-81-7P**
280752-13-8P 280752-14-9P 280752-36-5P
381229-64-7P 381229-66-9P 381229-67-0P
381229-69-2P 381229-70-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-activity relationships of p-arylthio cinnamides as antagonists of LFA-1/ICAM-1)
RN 280749-37-3 CAPLUS
CN Morpholine, 4-[(2E)-3-[3-chloro-4-[(2-methoxyphenyl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Welcome to STN International! Enter x:x

LOGINID:ssspta1611sxp

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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NEWS 7	OCT 21	BIOSIS file reloaded and enhanced
NEWS 8	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
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NEWS 11	DEC 08	IMS file names changed
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NEWS 21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS 22	FEB 05	German (DE) application and patent publication number format changes

NEWS EXPRESS	DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
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FILE 'HOME' ENTERED AT 16:41:54 ON 01 MAR 2004

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:42:11 ON 01 MAR 2004
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STRUCTURE FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9
DICTIONARY FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\09541795.13

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 16:42:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 441 TO ITERATE

100.0% PROCESSED 441 ITERATIONS 106 ANSWERS
SEARCH TIME: 00.00.01

L2 106 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 16:42:50 ON 01 MAR 2004

FILE COVERS 1907 - 1 Mar 2004 VOL 140 ISS 10
FILE LAST UPDATED: 29 Feb 2004 (20040229/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l2
L3            4 L2

=> d l3 fbib hitstr abs total

L3   ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:235035  CAPLUS
DN   139:285618
TI   QSAR Study on Some p-Arylthio Cinnamides as Antagonists of Biochemical
     ICAM-1/LFA-1 Interaction and ICAM-1/JY-8 Cell Adhesion in Relation to
     Anti-inflammatory Activity
AU   Debnath, Bikash; Samanta, Soma; Roy, Kunal; Jha, Tarun
CS   Department of Pharmaceutical Technology, Division of Pharmaceutical and
     Medicinal Chemistry, Jadavpur University, Kolkata, 700 032, India
SO   Bioorganic & Medicinal Chemistry (2003), 11(8), 1615-1619
     CODEN: BMECEP; ISSN: 0968-0896
PB   Elsevier Science Ltd.
DT   Journal
LA   English
IT   609841-80-7 609841-90-9 609841-91-0
     609841-95-4 609841-96-5 609841-97-6
     609842-01-5 609842-02-6 609842-03-7
     RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic
     use); BIOL (Biological study); USES (Uses)
        (QSAR study on arylthio cinnamides as antagonists of biochem.
        ICAM-1/LFA-1 interaction and ICAM-1/JY-8 cell adhesion)
RN   609841-80-7  CAPLUS
CN   Morpholine, 4-[3-[3-chloro-4-[(2-methoxyphenyl)thio]phenyl]-1-oxo-2-
     propenyl]- (9CI)  (CA INDEX NAME)
```

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 9	NOV 24	MSDS-CCOHS file reloaded
NEWS 10	DEC 08	CABA reloaded with left truncation
NEWS 11	DEC 08	IMS file names changed
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NEWS 19	DEC 22	ABI-INFORM now available on STN
NEWS 20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS 21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS 22	FEB 05	German (DE) application and patent publication number format changes

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FILE 'HOME' ENTERED AT 16:49:54 ON 01 MAR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:50:03 ON 01 MAR 2004
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STRUCTURE FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9
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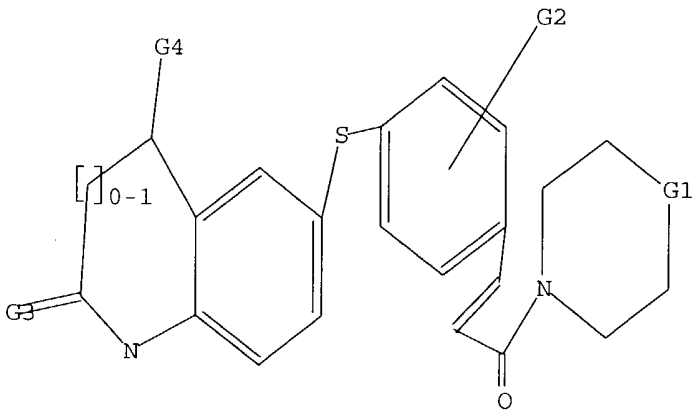
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\09541795.16

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,O,S,N,NH,CH2,CH

G2 CF3,X

G3 H,O

G4 C,O,S,N,CH2,CH

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 16:50:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 48 TO ITERATE

100.0% PROCESSED 48 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1

=> file marpat

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'MARPAT' ENTERED AT 16:50:39 ON 01 MAR 2004
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FILE CONTENT: 1988-PRESENT (VOL 140 ISS 09)(20040227/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6683216 27 JAN 2004
DE 10317487 05 FEB 2004
EP 1388584 11 FEB 2004
JP 2004035475 05 FEB 2004
WO 2004009876 29 JAN 2004

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

```
=> s l1 sss full
FULL SEARCH INITIATED 16:50:47 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED -   4167 TO ITERATE

100.0% PROCESSED    4167 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.18

L3            0 SEA SSS FUL L1

=> file caold
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             109.42     265.05

FILE 'CAOLD' ENTERED AT 16:51:12 ON 01 MAR 2004
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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  This file supports REG1stRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

=> s l1 sss full
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



FULL SEARCH INITIATED 16:51:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     48 TO ITERATE

100.0% PROCESSED      48 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.01

L4            0 SEA SSS FUL L1


L5            0 L4

=> log y
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
```

FULL ESTIMATED COST 0.42 421.31

STN INTERNATIONAL LOGOFF AT 16:51:28 ON 01 MAR 2004

Welcome to STN International! Enter x:x

LOGINID:ssspta1611sxp

PASSWORD:
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NEWS 16	DEC 19	CROPU no longer updated; subscriber discount no longer available
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NEWS 22	FEB 05	German (DE) application and patent publication number format changes

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FILE 'HOME' ENTERED AT 16:54:38 ON 01 MAR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:54:47 ON 01 MAR 2004
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STRUCTURE FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9
DICTIONARY FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9

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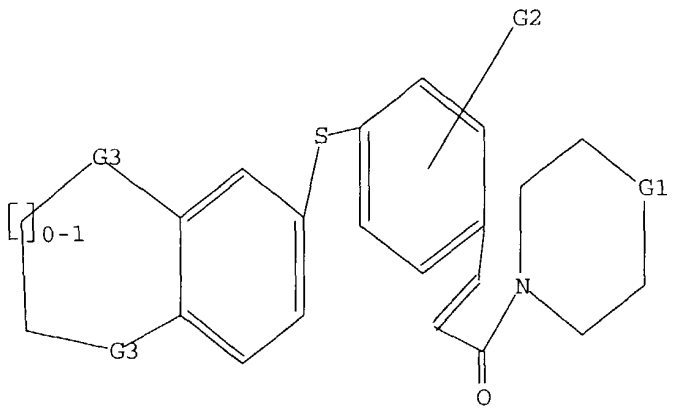
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\09541795.17

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,O,S,N,NH,CH2,CH

G2 CF3,X

G3 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sss full
FULL SEARCH INITIATED 16:55:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    610 TO ITERATE

100.0% PROCESSED     610 ITERATIONS                          67 ANSWERS
SEARCH TIME: 00.00.01

L2            67 SEA SSS FUL L1

=> file marpat
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             155.42     155.63

FILE 'MARPAT' ENTERED AT 16:55:26 ON 01 MAR 2004
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FILE CONTENT: 1988-PRESENT (VOL 140 ISS 09)(20040227/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US     6683216 27 JAN 2004
DE    10317487 05 FEB 2004
EP     1388584 11 FEB 2004
JP 2004035475 05 FEB 2004
WO 2004009876 29 JAN 2004

Structure search limits have been raised.  See HELP SLIMIT for the new,
higher limits.
```

```
=> s l1 sss full
FULL SEARCH INITIATED 16:55:34 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED -   8802 TO ITERATE

 93.2% PROCESSED    8204 ITERATIONS                                 1 ANSWERS

100.0% PROCESSED    8802 ITERATIONS                                 1 ANSWERS
SEARCH TIME: 00.00.24

L3             1 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     109.42     265.05

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FILE LAST UPDATED: 29 Feb 2004  (20040229/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> d his

     (FILE 'HOME' ENTERED AT 16:54:38 ON 01 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 16:54:47 ON 01 MAR 2004
L1               STRUCTURE UPLOADED
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     FILE 'MARPAT' ENTERED AT 16:55:26 ON 01 MAR 2004
L3             1 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 16:56:08 ON 01 MAR 2004

=> s l2
L4             6 L2

=> s l3
L5             1 L3
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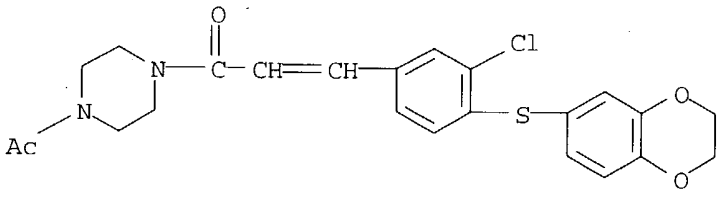
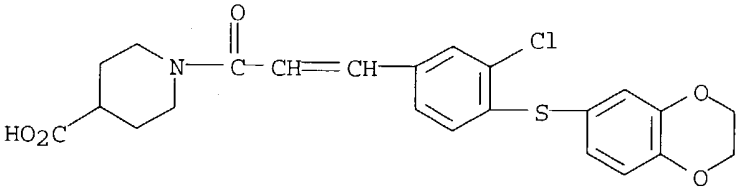
=> d l4 fbib hitstr abs total

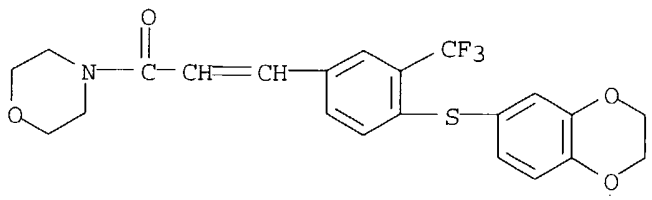
L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:235035 CAPLUS
DN 139:285618
TI QSAR Study on Some p-Arylthio Cinnamides as Antagonists of Biochemical ICAM-1/LFA-1 Interaction and ICAM-1/JY-8 Cell Adhesion in Relation to Anti-inflammatory Activity
AU Debnath, Bikash; Samanta, Soma; Roy, Kunal; Jha, Tarun
CS Department of Pharmaceutical Technology, Division of Pharmaceutical and Medicinal Chemistry, Jadavpur University, Kolkata, 700 032, India
SO Bioorganic & Medicinal Chemistry (2003), 11(8), 1615-1619
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
IT **609841-81-8 609841-82-9 609841-83-0**
609841-84-1 609841-85-2 609841-89-6
609841-93-2 609841-94-3 609841-98-7
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR study on arylthio cinnamides as antagonists of biochem. ICAM-1/LFA-1 interaction and ICAM-1/JY-8 cell adhesion)
RN 609841-81-8 CAPLUS
CN Piperazine, 1-acetyl-4-[3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



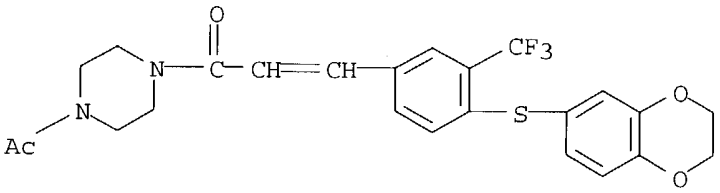
RN 609841-82-9 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



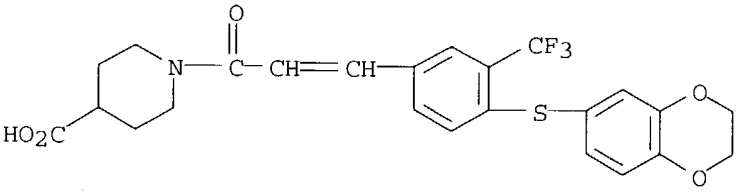
RN 609841-83-0 CAPLUS
CN Morpholine, 4-[3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



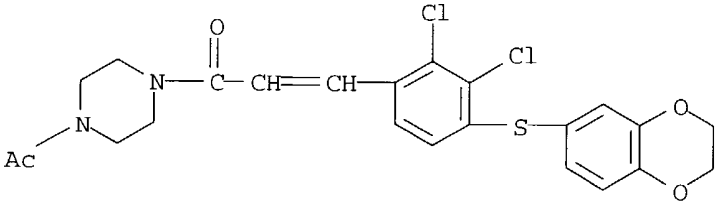
RN 609841-84-1 CAPLUS
CN Piperazine, 1-acetyl-4-[3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



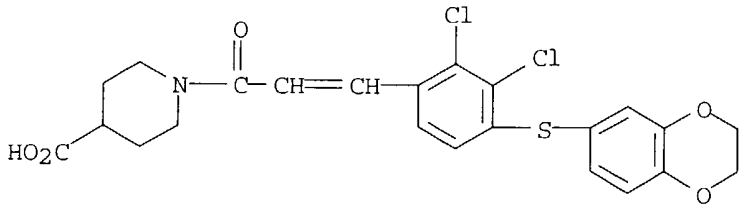
RN 609841-85-2 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



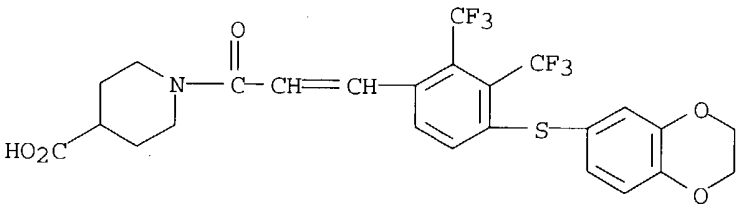
RN 609841-89-6 CAPLUS
CN Piperazine, 1-acetyl-4-[3-[2,3-dichloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



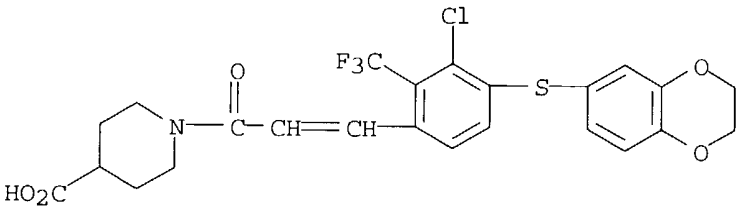
RN 609841-93-2 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[2,3-dichloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 609841-94-3 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-2,3-bis(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 609841-98-7 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-2-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



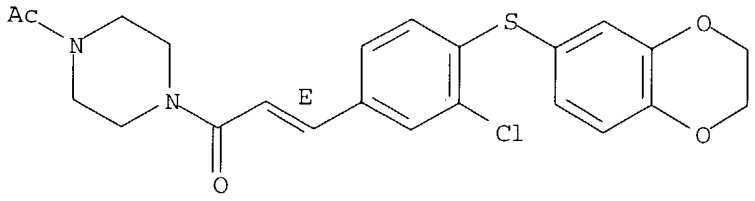
AB To find out the chemical and structural features of some p-arylthio cinnamides 1 as antagonists of biochem. ICAM-1/LFA-1 interaction as well as ICAM-1/JY-8 cell adhesion in relation to anti-inflammatory activity, QSAR study was performed. Steric effect on the arylthio ring and lipophilic substitutions at 2,3-positions, especially 2,3-disubstitution with Cl or CF3 or both on cinnamides 1 were conducive to the activity, whereas simultaneous presence of methoxy group at arylthio ring and NCOCH3 group at heterocyclic ring of cinnamides 1 were detrimental to activity in antagonism of biochem. ICAM-1/LFA-1 interaction. When inhibition of ICAM-1/JY-8 cell adhesion was considered, lipophilic substitution on ring B and simultaneous presence of CF3 groups at 2 and 3 positions of the ring B were advantageous to antagonism. This QSAR study showed that B ring has played the most important role for both types of activities.

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

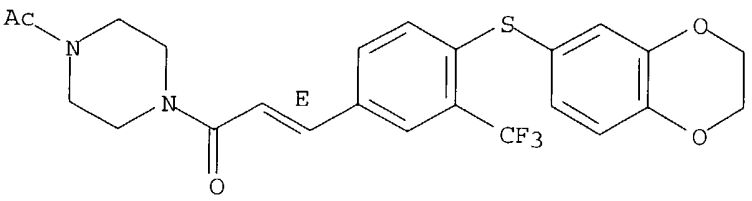
AN 2001:758465 CAPLUS
DN 136:47984
TI Discovery of Novel p-Arylthio Cinnamides as Antagonists of Leukocyte Function-Associated Antigen-1/Intercellular Adhesion Molecule-1 Interaction. 4. Structure-Activity Relationship of Substituents on the Benzene Ring of the Cinnamide
AU Winn, Martin; Reilly, Edward B.; Liu, Gang; Huth, Jeffrey R.; Jae, Hwan-Soo; Freeman, Jennifer; Pei, Zhonghua; Xin, Zhili; Lynch, John; Kester, Jeff; von Geldern, Thomas W.; Leitza, Sandra; DeVries, Peter; Dickinson, Robert; Mussatto, Donna; Okasinski, Gregory F.
CS Metabolic Disease Research Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064-6098, USA
SO Journal of Medicinal Chemistry (2001), 44(25), 4393-4403
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
IT **280750-31-4P 280750-96-1P 280751-25-9P**
280751-88-4P 280751-92-0P 280752-20-7P
301178-60-9P 381229-59-0P 381229-62-5P
381229-65-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-activity relationships of p-arylthio cinnamides as antagonists of LFA-1/ICAM-1)
RN 280750-31-4 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 280750-96-1 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

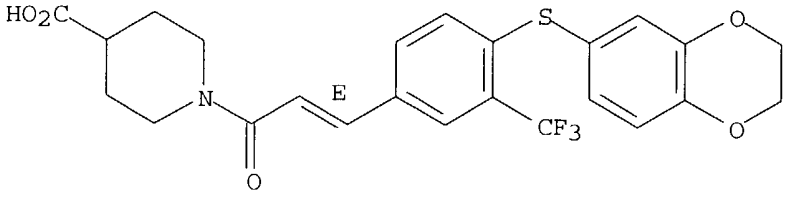
Double bond geometry as shown.



RN 280751-25-9 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-

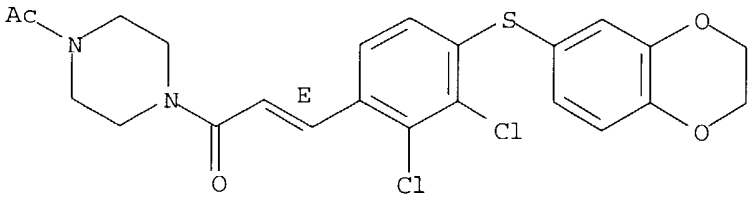
yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



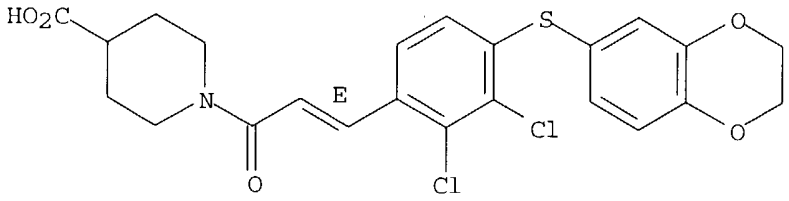
RN 280751-88-4 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[2,3-dichloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



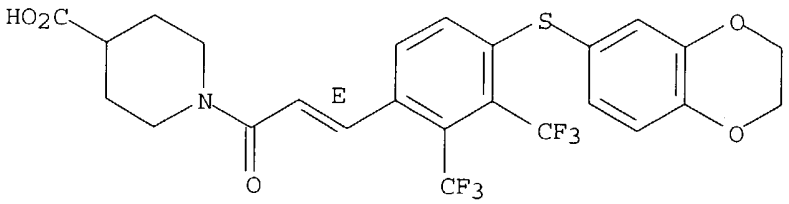
RN 280751-92-0 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[2,3-dichloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



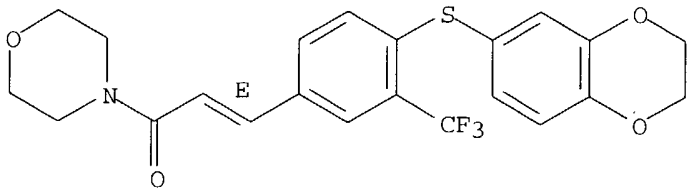
RN 280752-20-7 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-2,3-bis(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



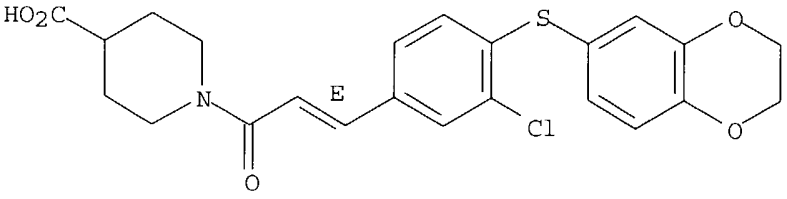
RN 301178-60-9 CAPLUS
CN Morpholine, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



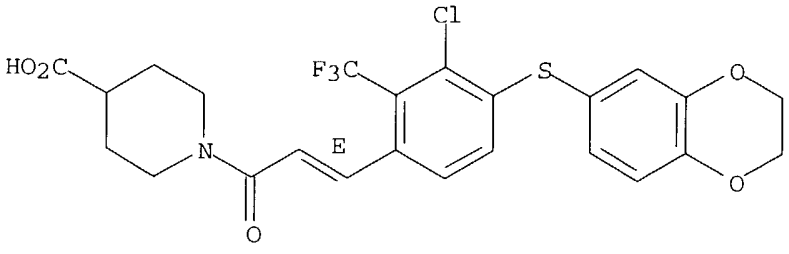
RN 381229-59-0 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



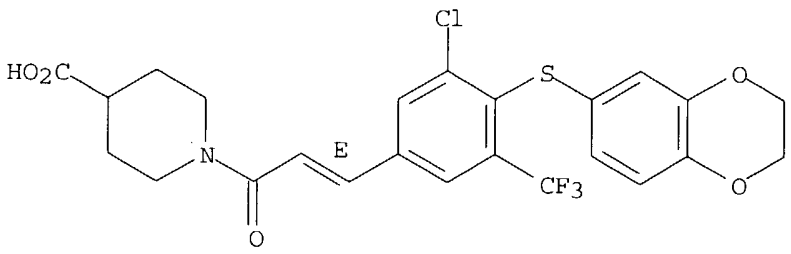
RN 381229-62-5 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-2-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 381229-65-8 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-5-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

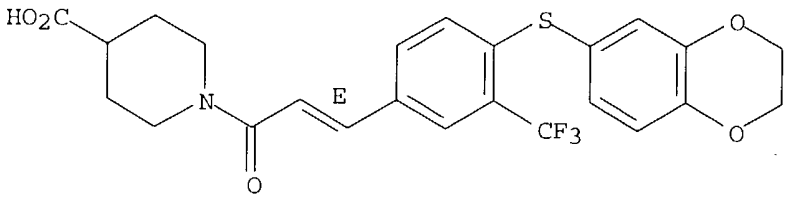


AB We have shown that p-arylthio cinnamides can inhibit the interaction of LFA-1 and ICAM-1, which is involved in cell adhesion and the inflammatory process. We now show that 2,3-disubstitution on the aryl portion of the cinnamide results in enhanced activity over mono substitution on the ring. The best 2,3-substituents were chlorine and trifluoromethyl groups. Compds. 39 and 40 which contain two CF3 groups have IC50 values of 0.5 and 0.1 nM, resp., in inhibiting JY8 cells expressing LFA-1 on their surface, from adhering to ICAM-1. The structure-activity relation (SAR) was examined using an NMR based model of the LFA-1 I domain/compound 31 complex. One of our compds. (38) was able to reduce cell migration in two different in vivo expts.

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

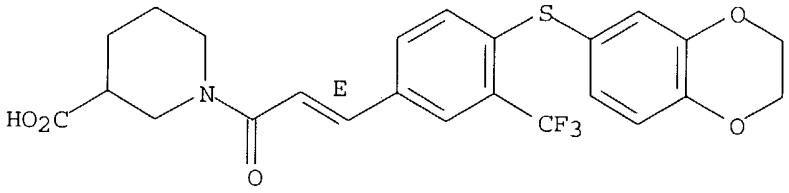
L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:555592 CAPLUS
DN 135:282681
TI Discovery of Potent Antagonists of Leukocyte Function-Associated Antigen-1/Intercellular Adhesion Molecule-1 Interaction. 3. Amide (C-Ring) Structure-Activity Relationship and Improvement of Overall Properties of Arylthio Cinnamides
AU Pei, Zhonghua; Xin, Zhili; Liu, Gang; Li, Yihong; Reilly, Edward B.; Lubbers, Nathan L.; Huth, Jeffery R.; Link, James T.; von Geldern, Thomas W.; Cox, Bryan F.; Leitza, Sandra; Gao, Yi; Marsh, Kennan C.; DeVries, Peter; Okasinski, Greg F.
CS Departments of Metabolic Disease Research Integrative Pharmacology Advanced Technology and Drug Analysis Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064, USA
SO Journal of Medicinal Chemistry (2001), 44(18), 2913-2920
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
IT **280751-25-9P 364613-14-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(discovery of potent antagonists of LFA-1/ICAM-1 interaction. 3. amide SAR and improvement of overall properties of arylthio cinnamides)
RN 280751-25-9 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 364613-14-9 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



AB The interaction of LFA-1 and ICAM-1 plays an important role in the cell adhesion process. On the basis of previously reported SAR and structural information on the binding of our p-arylthiocinnamide series to LFA-1, we have identified the cyclic amide (C-ring) as a site for modification. Improvement in potency and, more importantly, in the phys. properties and pharmacokinetic profiles of the leading compds. resulted from this modification. One of the best compds. (11f) is also shown to reduce myocardial infarct size in rat.
RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

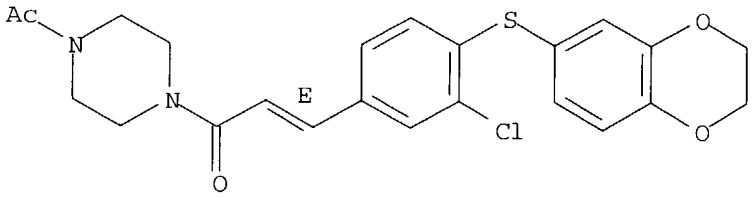
L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:192987 CAPLUS
DN 135:160
TI Novel p-Arylthio Cinnamides as Antagonists of Leukocyte Function-Associated Antigen-1/Intracellular Adhesion Molecule-1 Interaction. 2. Mechanism of Inhibition and Structure-Based Improvement of Pharmaceutical Properties
AU Liu, Gang; Huth, Jeffrey R.; Olejniczak, Edward T.; Mendoza, Renaldo; DeVries, Peter; Leitza, Sandra; Reilly, Edward B.; Okasinski, Gregory F.; Fesik, Stephen W.; von Geldern, Thomas W.
CS Metabolic Disease Research and Research NMR Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064-6098, USA
SO Journal of Medicinal Chemistry (2001), 44(8), 1202-1210
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 135:160
IT **280750-31-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation and structure activity relations of arylthiocinnamides as antagonists of antigen LFA-1/ICAM-1 interaction as derived from NMR based screening)

RN 280750-31-4 CAPLUS

CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

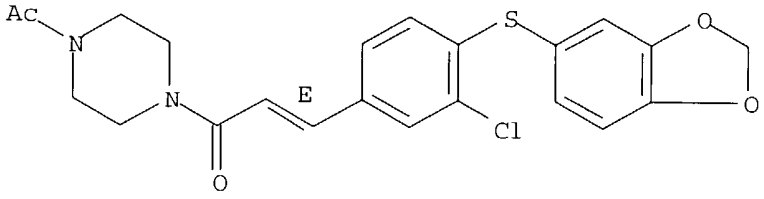


IT **280749-53-3P 280750-12-1P 280750-82-5P 280750-88-1P 280751-01-1P 280751-40-8P 341497-65-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure activity relations of arylthiocinnamides as antagonists of antigen LFA-1/ICAM-1 interaction as derived from NMR based screening)

RN 280749-53-3 CAPLUS

CN Piperazine, 1-acetyl-4-[(2E)-3-[4-(1,3-benzodioxol-5-ylthio)-3-chlorophenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

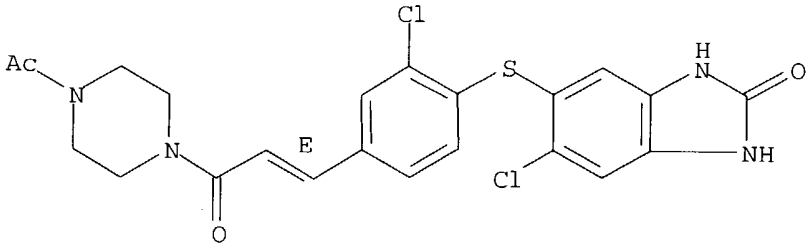
Double bond geometry as shown.



RN 280750-12-1 CAPLUS

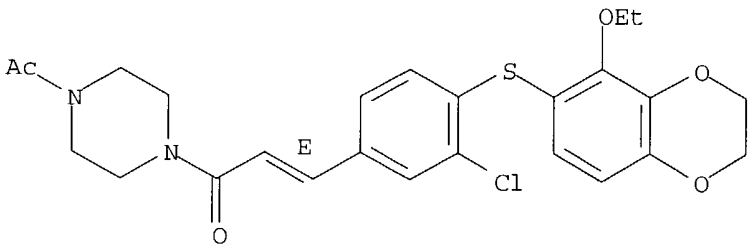
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[(6-chloro-2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



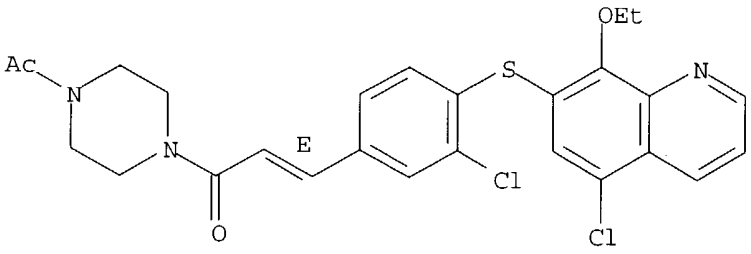
RN 280750-82-5 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[(5-ethoxy-2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



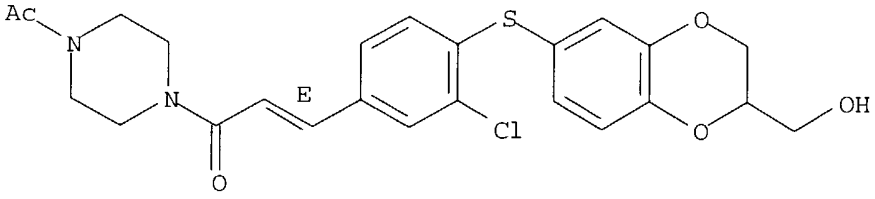
RN 280750-88-1 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[(5-chloro-8-ethoxy-7-quinolinyl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



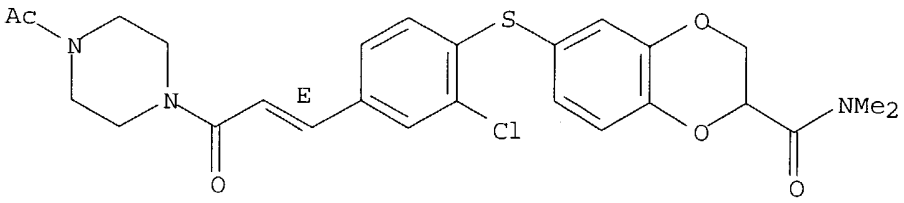
RN 280751-01-1 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[[2,3-dihydro-2-(hydroxymethyl)-1,4-benzodioxin-6-yl]thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



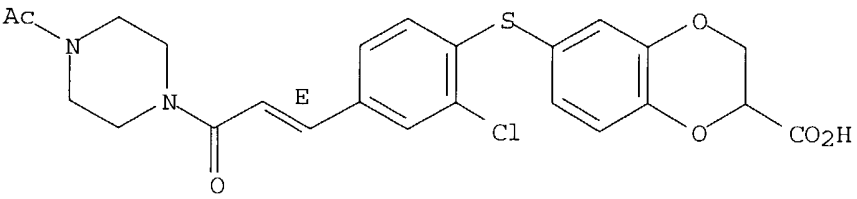
RN 280751-40-8 CAPLUS
CN 1,4-Benzodioxin-2-carboxamide, 6-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propenyl]-2-chlorophenyl]thio]-2,3-dihydro-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 341497-65-2 CAPLUS
CN 1,4-Benzodioxin-2-carboxylic acid, 6-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propenyl]-2-chlorophenyl]thio]-2,3-dihydro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



AB The interaction between leukocyte function-associated antigen-1 (LFA-1) and intracellular adhesion mol.-1 (ICAM-1) has been implicated in inflammatory and immune diseases. Recently, a novel series of p-arylthio cinnamides has been described as potent antagonists of the LFA-1/ICAM-1 interaction. These compds. were found to bind to the I domain of LFA-1 using two-dimensional NMR spectroscopy of 15N-labeled LFA-1 I domain. On the basis of NOE studies between a certain compound and the I domain of LFA-1, a model of the complex was constructed. This model revealed that this compound does not directly inhibit ICAM-1 binding by interacting with the metal ion dependent adhesion site (MIDAS), Instead, it binds to the previously proposed I domain allosteric site (IDAS) of LFA-1 and likely modulates the activation of LFA-1 through its interaction with this regulatory site. A fragment-based NMR screening strategy was applied to identify small, more water-soluble ligands that bind to a specific region of the IDAS. When incorporated into the parent cinnamide template, the resulting analogs exhibited increased aqueous solubility and improved pharmacokinetic profiles in rats, demonstrating the power of this NMR-based screening approach for rapidly modifying high-affinity ligands.
RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:725609 CAPLUS
DN 133:296281
TI Preparation of 2- or 4-(phenylthio)cinnamides as cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds
IN Link, James; Liu, Gang; Pei, Zhonghua; Von Geldern, Thomas W.; Winn, Martin; Xin, Zhili; Wang, Sheldon; Boyd, Steven A.; Zhu, Gui-Dong; Freeman, Jennifer C.; Gunawardana, Indrani W.; Staeger, Michael A.; Jae, Hwan-soo; Lynch, John K.
PA Abbott Laboratories, USA
SO PCT Int. Appl., 476 pp.
CODEN: PIXXD2
DT Patent

LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000059880	A1	20001012	WO 2000-US8895	20000403
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
				US 1999-286645 A	19990402
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				WO 2000-US8895 W	20000403
	EE 200100513	A	20021216	EE 2001-513	20000403
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	BG 106029	A	20020531	BG 2001-106029	20011018
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				WO 2000-US8895 W	20000403
	HR 2001000776	A1	20021231	HR 2001-776	20011023
				US 1999-286645 A	19990402
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				US 2000-541795 A	20000331
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	ZA 2001008944	A	20030702	ZA 2001-8944	20011030
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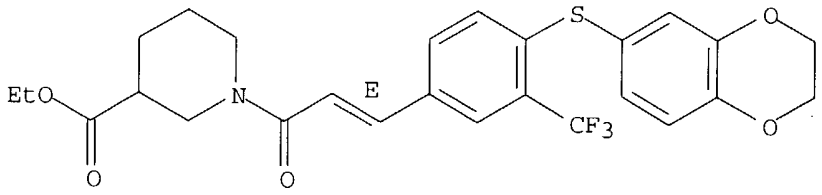
OS MARPAT 133:296281

IT **280751-10-2P 280751-11-3P 280751-14-6P**
280751-15-7P 280751-17-9P 280751-31-7P
280751-71-5P 280751-72-6P 280751-77-1P
280751-85-1P 280751-89-5P 280751-90-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

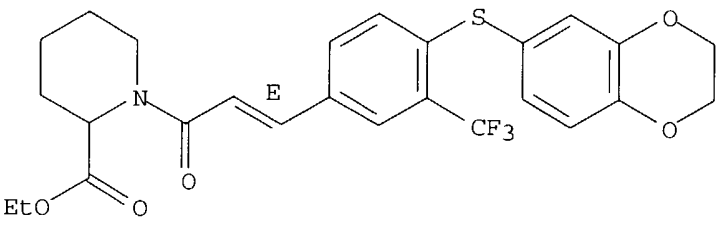
RN 280751-10-2 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



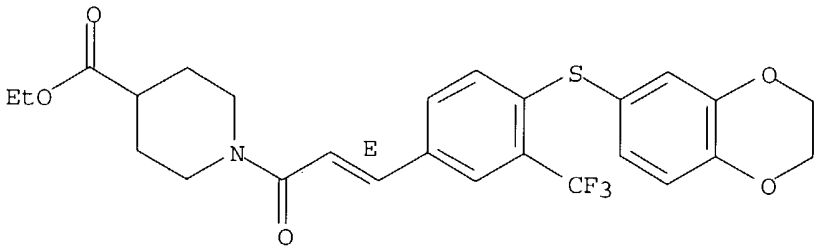
RN 280751-11-3 CAPLUS
CN 2-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



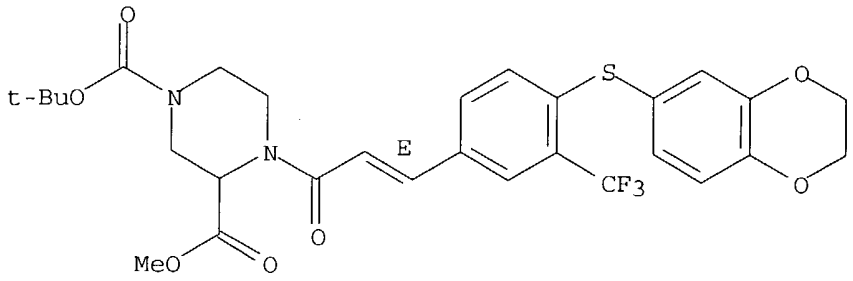
RN 280751-14-6 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



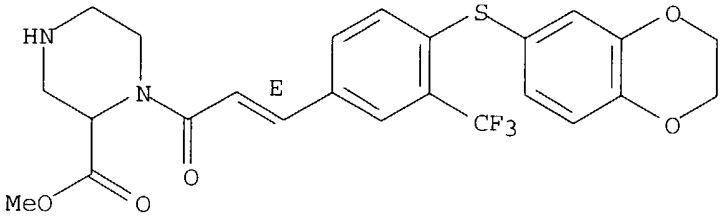
RN 280751-15-7 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, 1-(1,1-dimethylethyl) 3-methyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



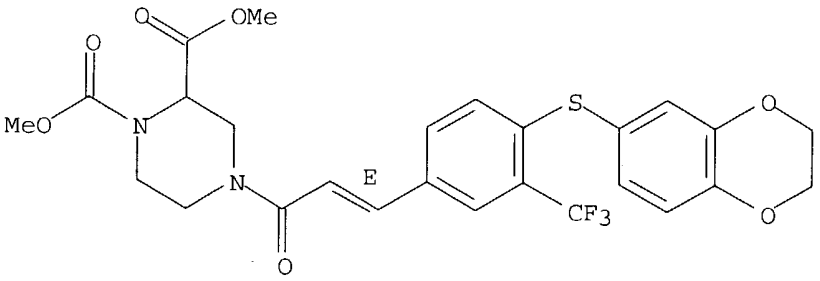
RN 280751-17-9 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, methyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



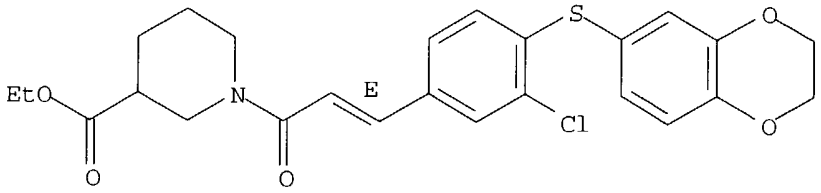
RN 280751-31-7 CAPLUS
CN 1,2-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



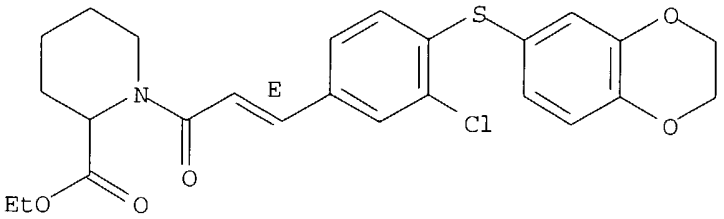
RN 280751-71-5 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



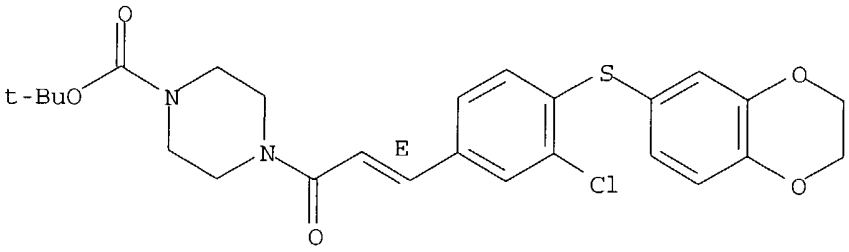
RN 280751-72-6 CAPLUS
CN 2-Piperidinecarboxylic acid, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



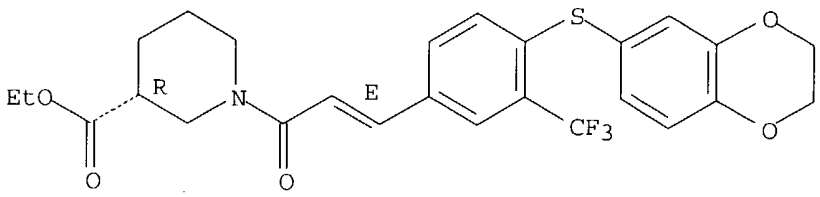
RN 280751-77-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



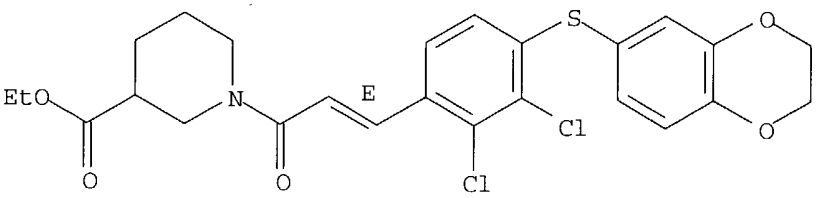
RN 280751-85-1 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, ethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



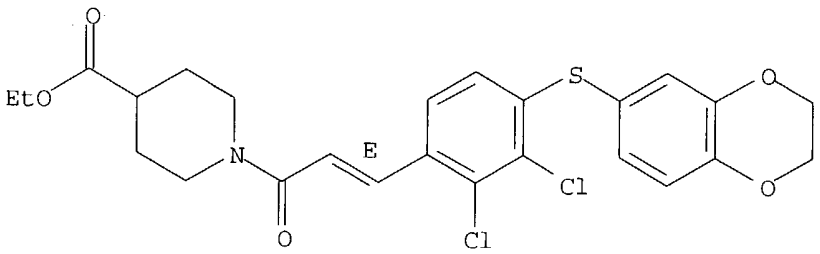
RN 280751-89-5 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[(2E)-3-[2,3-dichloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 280751-90-8 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[2,3-dichloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **280749-53-3P 280750-12-1P 280750-31-4P**
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280751-01-1P 280751-16-8P 280751-25-9P
280751-26-0P 280751-27-1P 280751-29-3P
280751-30-6P 280751-33-9P 280751-35-1P
280751-39-5P 280751-54-4P 280751-55-5P
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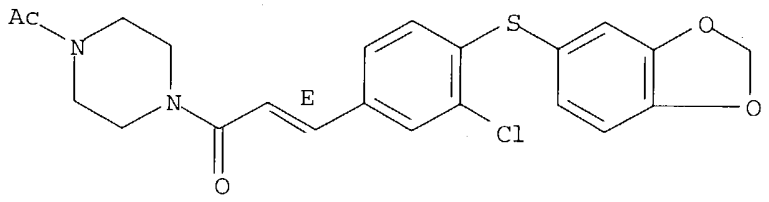
280753-36-8P 301178-60-9P 301178-61-0P
301178-62-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

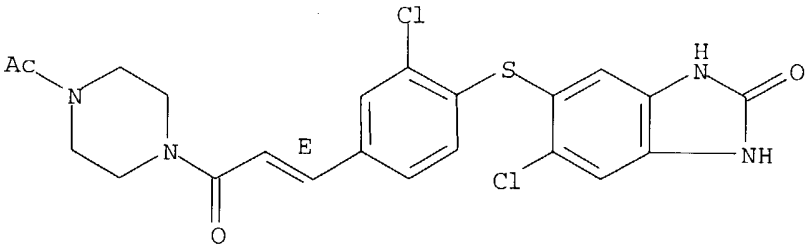
RN 280749-53-3 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[4-(1,3-benzodioxol-5-ylthio)-3-chlorophenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



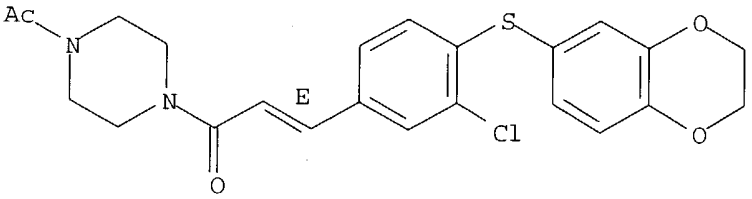
RN 280750-12-1 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[(6-chloro-2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



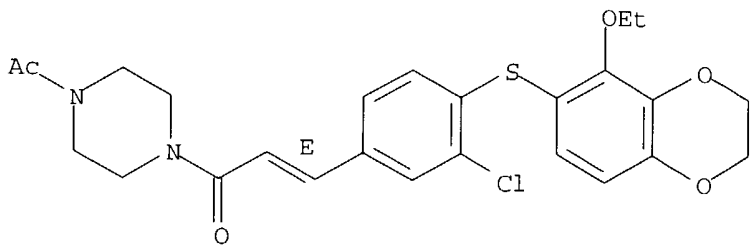
RN 280750-31-4 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



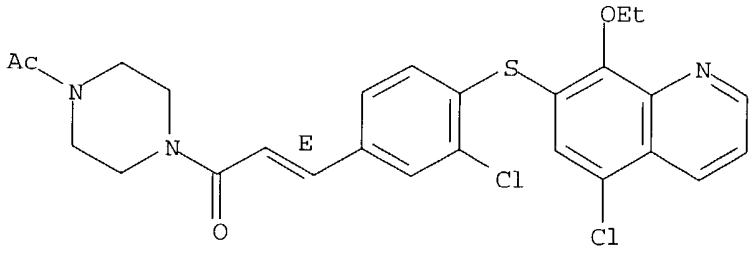
RN 280750-82-5 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[(5-ethoxy-2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



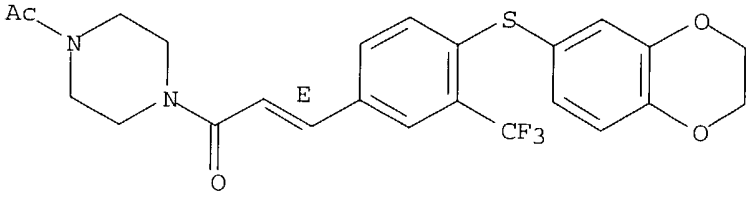
RN 280750-88-1 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[(5-chloro-8-ethoxy-7-quinolinyl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



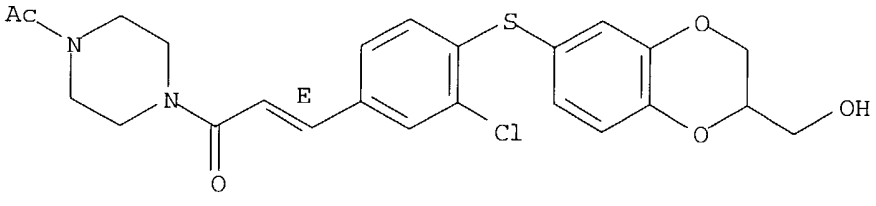
RN 280750-96-1 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



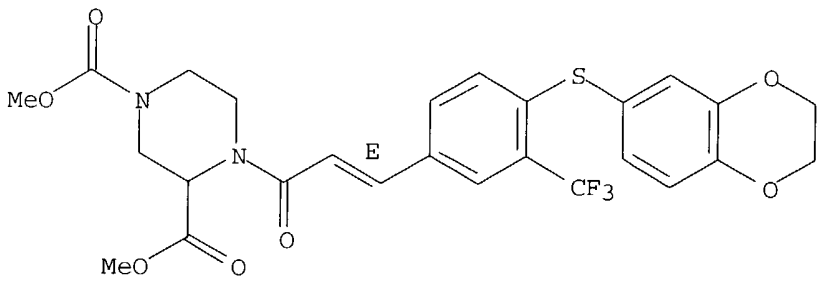
RN 280751-01-1 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[3-chloro-4-[[2,3-dihydro-2-(hydroxymethyl)-1,4-benzodioxin-6-yl]thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



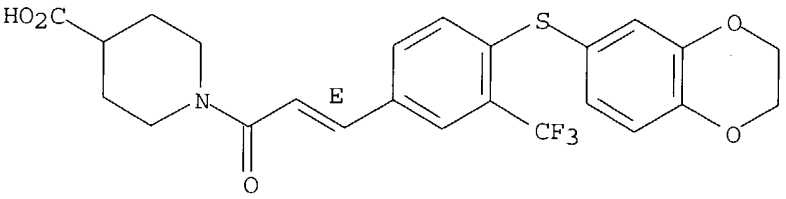
RN 280751-16-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



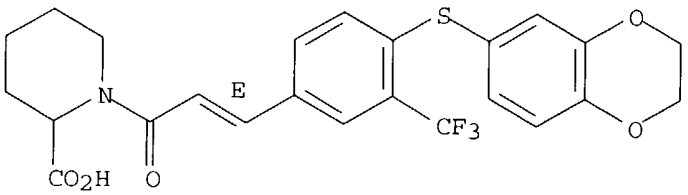
RN 280751-25-9 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



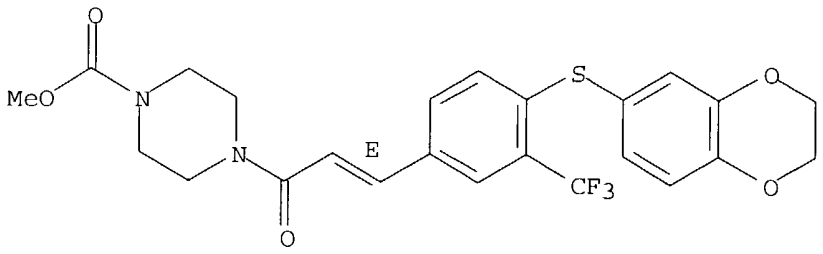
RN 280751-26-0 CAPLUS
CN 2-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



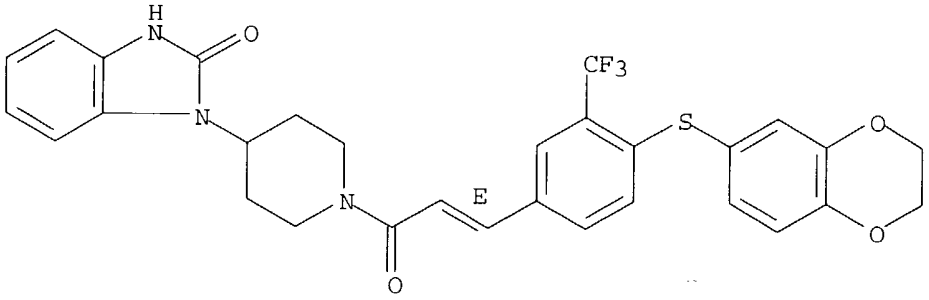
RN 280751-27-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, methyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



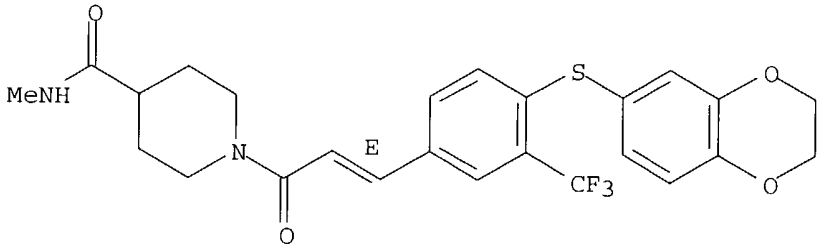
RN 280751-29-3 CAPLUS
CN Piperidine, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



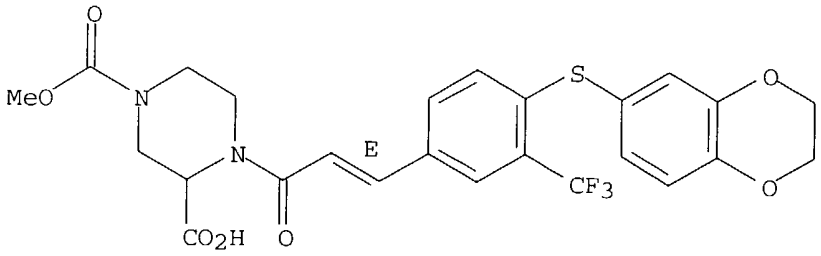
RN 280751-30-6 CAPLUS
CN 4-Piperidinecarboxamide, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-N-methyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



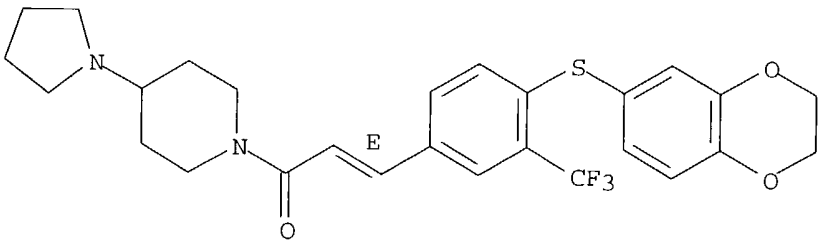
RN 280751-33-9 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, 1-methyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



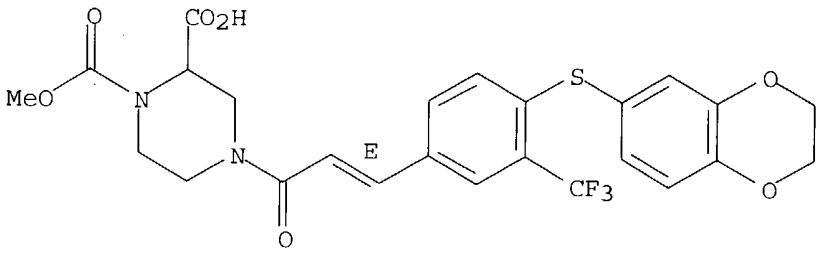
RN 280751-35-1 CAPLUS
CN Piperidine, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-4-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



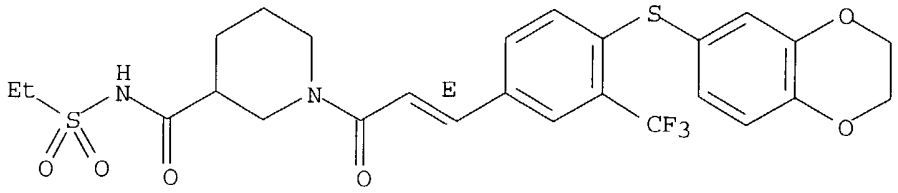
RN 280751-39-5 CAPLUS
CN 1,2-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, 1-methyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 280751-54-4 CAPLUS
CN 3-Piperidinecarboxamide, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-N-(ethylsulfonyl)- (9CI) (CA INDEX NAME)

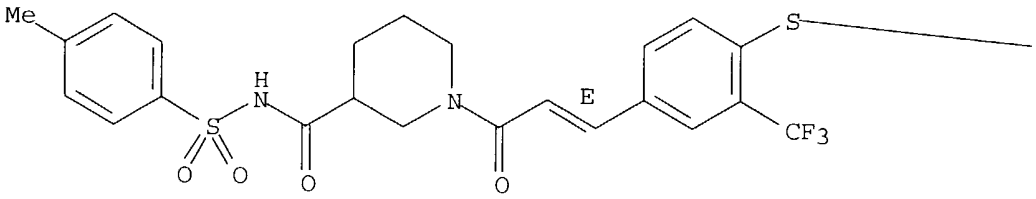
Double bond geometry as shown.



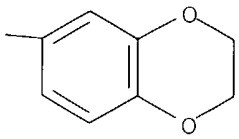
RN 280751-55-5 CAPLUS
CN 3-Piperidinecarboxamide, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

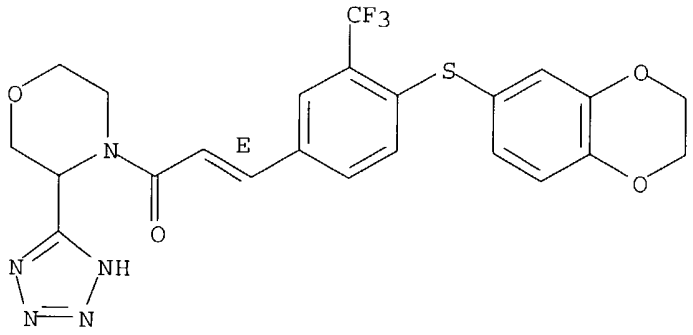


PAGE 1-B



RN 280751-57-7 CAPLUS
CN Morpholine, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-3-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

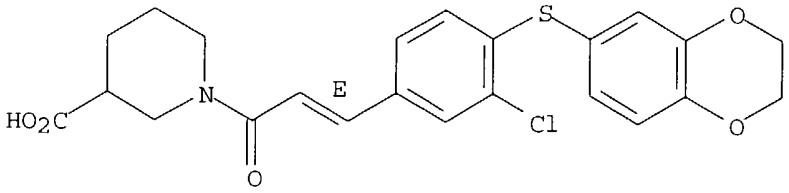
Double bond geometry as shown.



RN 280751-63-5 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-

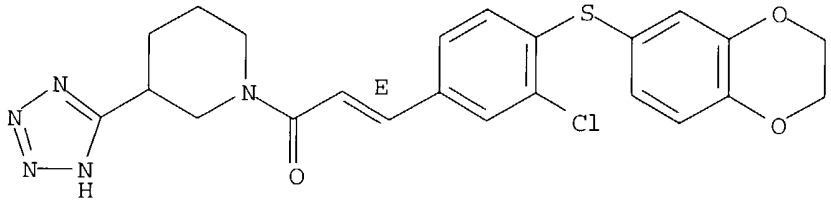
benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



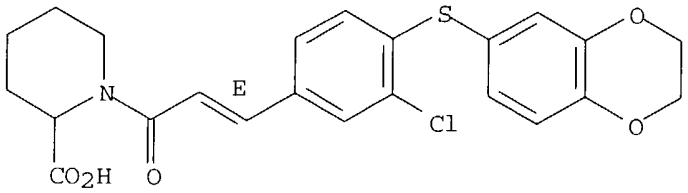
RN 280751-76-0 CAPLUS
CN Piperidine, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-3-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



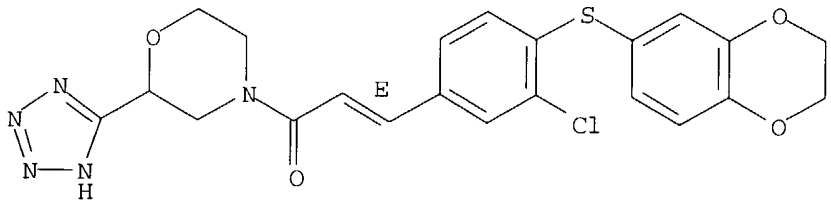
RN 280751-78-2 CAPLUS
CN 2-Piperidinecarboxylic acid, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



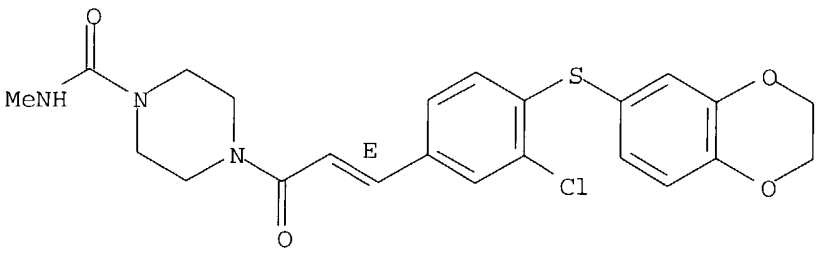
RN 280751-79-3 CAPLUS
CN Morpholine, 4-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-2-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



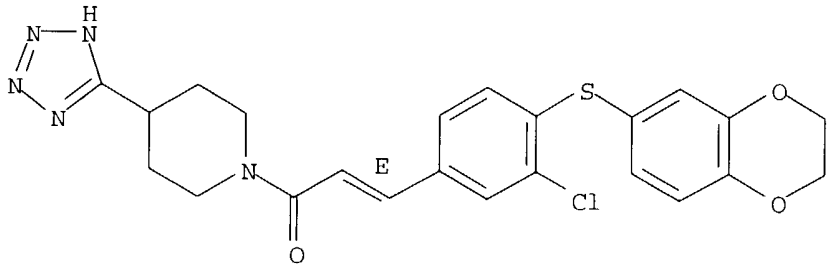
RN 280751-80-6 CAPLUS
CN 1-Piperazinecarboxamide, 4-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-N-methyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



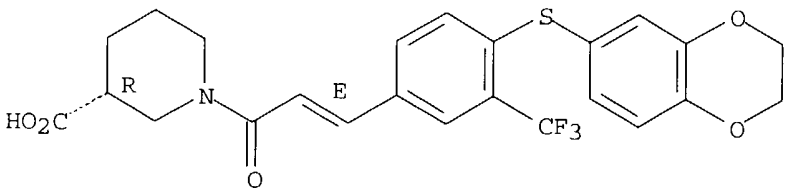
RN 280751-82-8 CAPLUS
CN Piperidine, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



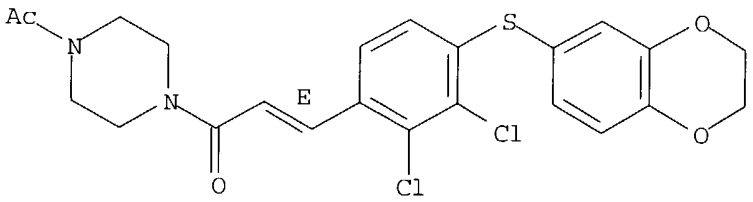
RN 280751-86-2 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



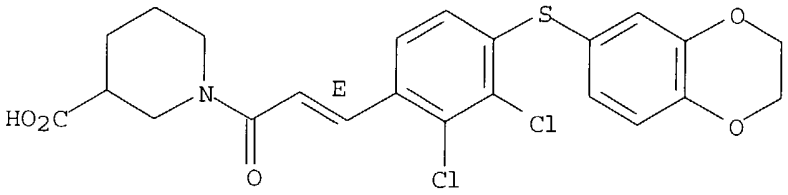
RN 280751-88-4 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[2,3-dichloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



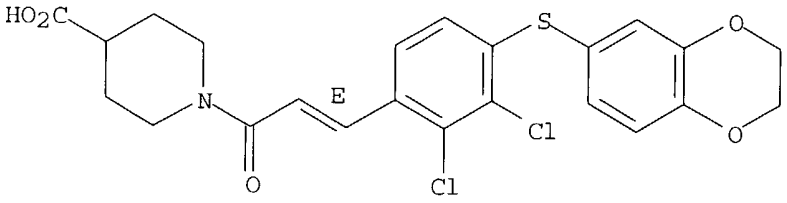
RN 280751-91-9 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[(2E)-3-[2,3-dichloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



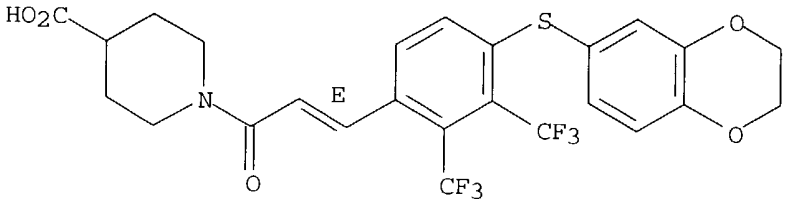
RN 280751-92-0 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[2,3-dichloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 280752-20-7 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-2,3-bis(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

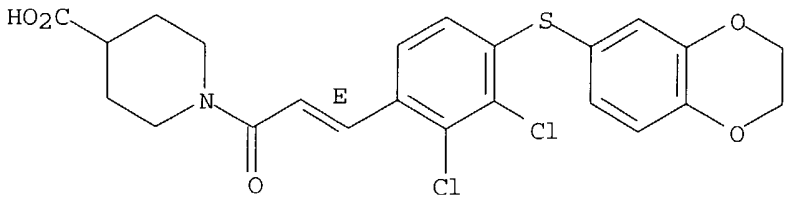
Double bond geometry as shown.



RN 280752-51-4 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[(2E)-3-[2,3-dichloro-4-[(2,3-dihydro-1,4-

benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-, sodium salt (9CI) (CA INDEX NAME)

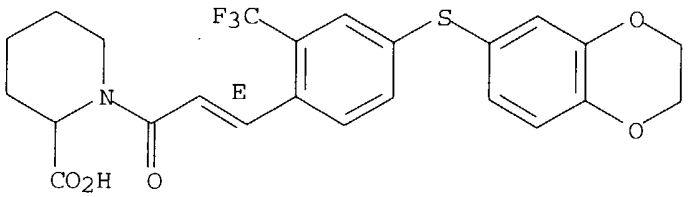
Double bond geometry as shown.



● Na

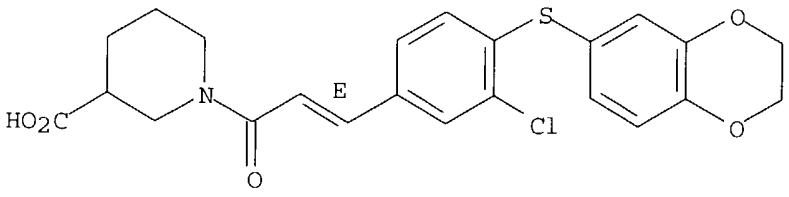
RN 280753-27-7 CAPLUS
CN 2-Piperidinecarboxylic acid, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-2-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 280753-35-7 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-, sodium salt (9CI) (CA INDEX NAME)

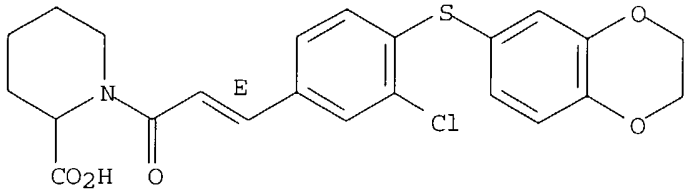
Double bond geometry as shown.



● Na

RN 280753-36-8 CAPLUS
CN 2-Piperidinecarboxylic acid, 1-[(2E)-3-[3-chloro-4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]phenyl]-1-oxo-2-propenyl]-, sodium salt (9CI) (CA INDEX NAME)

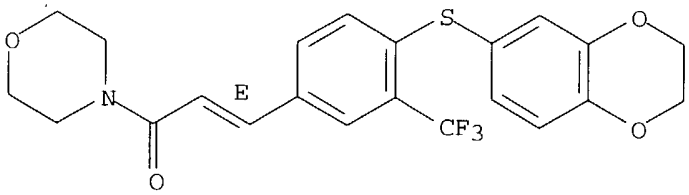
Double bond geometry as shown.



● Na

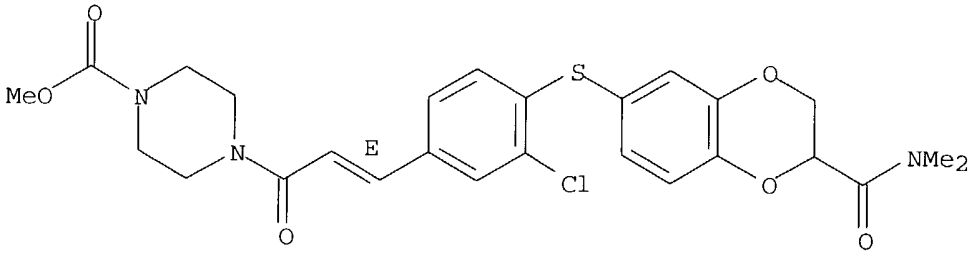
RN 301178-60-9 CAPLUS
CN Morpholine, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



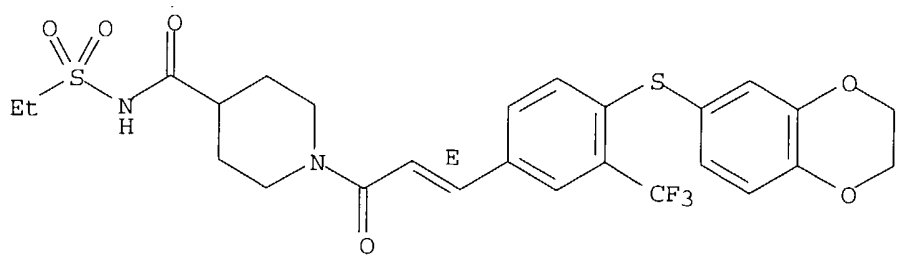
RN 301178-61-0 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[3-chloro-4-[[2-[(dimethylamino)carbonyl]-2,3-dihydro-1,4-benzodioxin-6-yl]thio]phenyl]-1-oxo-2-propenyl]-, methyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 301178-62-1 CAPLUS
CN 4-Piperidinecarboxamide, 1-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]-N-(ethylsulfonyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

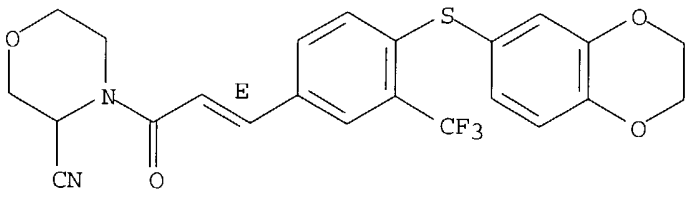


IT **301180-14-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

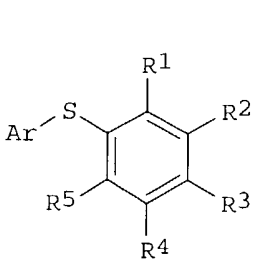
RN 301180-14-3 CAPLUS

CN 3-Morpholinecarbonitrile, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-(trifluoromethyl)phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

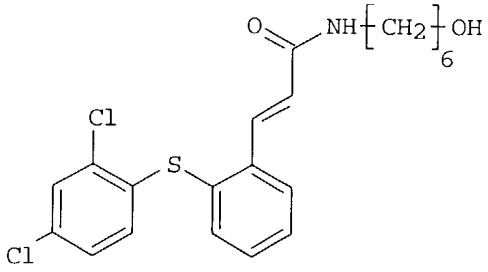
Double bond geometry as shown.



GI



I



II

AB The title compds. (I) [wherein R1-R5 = independently H, halo, (halo)alkyl, alkoxy, cyano, NO2, CHO, and least one of R1 or R3 is an (un)substituted cis- or trans-cinnamide; Ar = (un)substituted (hetero)aryl] were prepared as cell adhesion inhibitors for the treatment of inflammatory and immune diseases. Examples include syntheses for 443 invention compds. and data for 3 bioassays. For instance, a mixture of 2-[(2,4-dichlorophenyl)thio]benzaldehyde (preparation given), malonic acid, piperidine in anhydrous pyridine was heated at 110°C for 2 h and then treated with aqueous HCl to give trans-2-[(2,4-dichlorophenyl)thio]cinnamic acid (91%). Conversion to the acid chloride followed by amidation with

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NEWS 8	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
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NEWS 10	DEC 08	CABA reloaded with left truncation
NEWS 11	DEC 08	IMS file names changed
NEWS 12	DEC 09	Experimental property data collected by CAS now available in REGISTRY
NEWS 13	DEC 09	STN Entry Date available for display in REGISTRY and CA/CAplus
NEWS 14	DEC 17	DGENE: Two new display fields added
NEWS 15	DEC 18	BIOTECHNO no longer updated
NEWS 16	DEC 19	CROPU no longer updated; subscriber discount no longer available
NEWS 17	DEC 22	Additional INPI reactions and pre-1907 documents added to CAS databases
NEWS 18	DEC 22	IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19	DEC 22	ABI-INFORM now available on STN
NEWS 20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS 21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS 22	FEB 05	German (DE) application and patent publication number format changes
NEWS EXPRESS		DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
NEWS INTER		General Internet Information
NEWS LOGIN		Welcome Banner and News Items
NEWS PHONE		Direct Dial and Telecommunication Network Access to STN
NEWS WWW		CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:02:08 ON 01 MAR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:02:40 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9
DICTIONARY FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

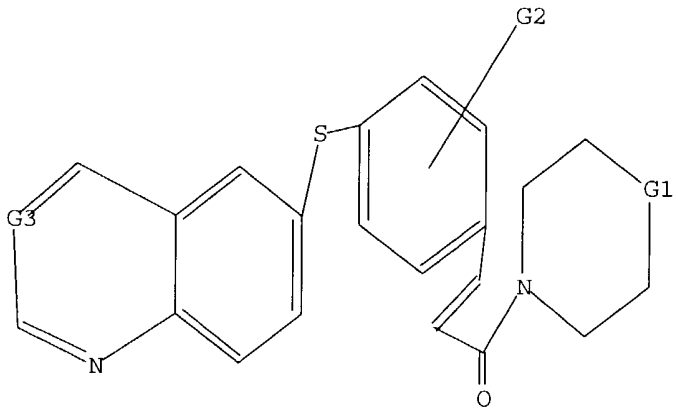
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\09541795.18

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,O,S,N,NH,CH2,CH

G2 CF3,X

G3 C,O,S,N,CH

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 17:03:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 63 TO ITERATE

100.0% PROCESSED 63 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1

=> file marpat

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'MARPAT' ENTERED AT 17:03:12 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE CONTENT: 1988-PRESENT (VOL 140 ISS 09)(20040227/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6683216 27 JAN 2004
DE 10317487 05 FEB 2004
EP 1388584 11 FEB 2004
JP 2004035475 05 FEB 2004
WO 2004009876 29 JAN 2004

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> s l1 sss full
FULL SEARCH INITIATED 17:03:18 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED - 4267 TO ITERATE

100.0% PROCESSED 4267 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.11

L3 0 SEA SSS FUL L1

=> file caold
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	109.42	265.05

FILE 'CAOLD' ENTERED AT 17:03:35 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s l1 sss full
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 17:03:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 63 TO ITERATE

100.0% PROCESSED 63 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L1

L5 0 L4

=> log y
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	421.31

STN INTERNATIONAL LOGOFF AT 17:03:48 ON 01 MAR 2004

Welcome to STN International! Enter x:x

LOGINID:ssspta1611sxp

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	SEP 09	CA/CAplus records now contain indexing from 1907 to the present
NEWS 4	DEC 08	INPADOC: Legal Status data reloaded
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NEWS 6	OCT 10	PCTFULL: Two new display fields added
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NEWS 9	NOV 24	MSDS-CCOHS file reloaded
NEWS 10	DEC 08	CABA reloaded with left truncation
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NEWS 21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS 22	FEB 05	German (DE) application and patent publication number format changes

NEWS EXPRESS	DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
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* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:06:11 ON 01 MAR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:06:23 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9
DICTIONARY FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

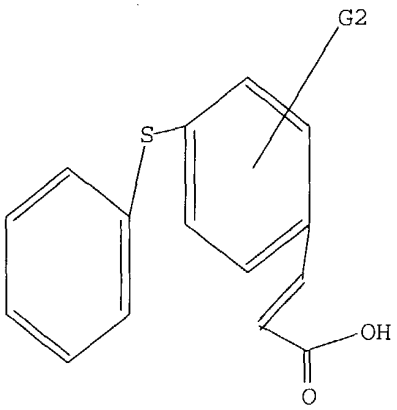
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\09541795.19

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,O,S,N,NH,CH2,CH

G2 CF3,X

G3 C,O,S,N,CH

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sss full
FULL SEARCH INITIATED 17:06:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    173 TO ITERATE

100.0% PROCESSED     173 ITERATIONS                          18 ANSWERS
SEARCH TIME: 00.00.01

L2            18 SEA SSS FUL L1

=> file marpat
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             155.42     155.63

FILE 'MARPAT' ENTERED AT 17:06:53 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

FILE CONTENT: 1988-PRESENT (VOL 140 ISS 09)(20040227/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US     6683216 27 JAN 2004
DE    10317487 05 FEB 2004
EP     1388584 11 FEB 2004
JP 2004035475 05 FEB 2004
WO 2004009876 29 JAN 2004

Structure search limits have been raised.  See HELP SLIMIT for the new,
higher limits.
```

=>

=> s l1 sss full
FULL SEARCH INITIATED 17:07:04 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED - 2146 TO ITERATE

99.6% PROCESSED 2137 ITERATIONS 17 ANSWERS

100.0% PROCESSED 2146 ITERATIONS 17 ANSWERS
SEARCH TIME: 00.00.18

L3 17 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 109.42 265.05

FILE 'CAPLUS' ENTERED AT 17:07:28 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 1 Mar 2004 VOL 140 ISS 10
FILE LAST UPDATED: 29 Feb 2004 (20040229/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 17:06:11 ON 01 MAR 2004)

FILE 'REGISTRY' ENTERED AT 17:06:23 ON 01 MAR 2004
L1 STRUCTURE UPLOADED
L2 18 S L1 SSS FULL

FILE 'MARPAT' ENTERED AT 17:06:53 ON 01 MAR 2004
L3 17 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 17:07:28 ON 01 MAR 2004

=> s l2
L4 5 L2

=> s l3

Welcome to STN International! Enter x:x

LOGINID:ssspta1611sxp

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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NEWS 15	DEC 18	BIOTECHNO no longer updated
NEWS 16	DEC 19	CROPU no longer updated; subscriber discount no longer available
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NEWS 20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
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NEWS 22	FEB 05	German (DE) application and patent publication number format changes

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FILE 'HOME' ENTERED AT 17:14:25 ON 01 MAR 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:14:34 ON 01 MAR 2004
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STRUCTURE FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9
DICTIONARY FILE UPDATES: 29 FEB 2004 HIGHEST RN 656221-41-9

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

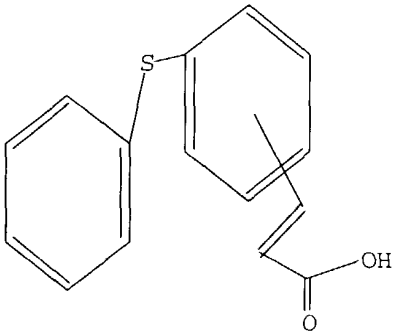
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading c:\program files\stnexp\queries\09541795.20

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,O,S,N,NH,CH2,CH

G2 CF3,X

G3 C,O,S,N,CH

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 17:14:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 687 TO ITERATE

100.0% PROCESSED 687 ITERATIONS 86 ANSWERS
SEARCH TIME: 00.00.01

L2 86 SEA SSS FUL L1

=> file marpat

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'MARPAT' ENTERED AT 17:15:06 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

FILE CONTENT: 1988-PRESENT (VOL 140 ISS 09)(20040227/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6683216 27 JAN 2004
DE 10317487 05 FEB 2004
EP 1388584 11 FEB 2004
JP 2004035475 05 FEB 2004
WO 2004009876 29 JAN 2004

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> s l1 sss full
FULL SEARCH INITIATED 17:15:12 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED - 3971 TO ITERATE

98.3% PROCESSED 3902 ITERATIONS 43 ANSWERS

99.4% PROCESSED 3946 ITERATIONS (1 INCOMPLETE) 45 ANSWERS

100.0% PROCESSED 3971 ITERATIONS (1 INCOMPLETE) 45 ANSWERS
SEARCH TIME: 00.00.43

L3 45 SEA SSS FUL L1

=> file caold
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST 109.84 265.47

FILE 'CAOLD' ENTERED AT 17:16:02 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGlstRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s lll sss full
L4 0 LL1

=> s l1 sss full
REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 17:16:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 687 TO ITERATE

100.0% PROCESSED 687 ITERATIONS 86 ANSWERS
SEARCH TIME: 00.00.01

L5 86 SEA SSS FUL L1

L6 1 L5

```
=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.42     423.46

FILE 'CAPLUS' ENTERED AT 17:16:39 ON 01 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 1 Mar 2004  VOL 140 ISS 10
FILE LAST UPDATED: 29 Feb 2004  (20040229/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> d his

     (FILE 'HOME' ENTERED AT 17:14:25 ON 01 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 17:14:34 ON 01 MAR 2004
L1              STRUCTURE UPLOADED
L2           86 S L1 SSS FULL

     FILE 'MARPAT' ENTERED AT 17:15:06 ON 01 MAR 2004
L3           45 S L1 SSS FULL

     FILE 'CAOLD' ENTERED AT 17:16:02 ON 01 MAR 2004
L4            0 S LL1 SSS FULL
                S L1

     FILE 'REGISTRY' ENTERED AT 17:16:27 ON 01 MAR 2004
L5           86 S L1 SSS FULL

     FILE 'CAOLD' ENTERED AT 17:16:27 ON 01 MAR 2004
L6            1 S L5 SSS FULL

     FILE 'CAPLUS' ENTERED AT 17:16:39 ON 01 MAR 2004

=> s l2
L7           22 L2

=> s l3
L8           45 L3

=> s l 6
```

```
L9        2306 L 6

=> s l6
L10         22 L5

=> d his

     (FILE 'HOME' ENTERED AT 17:14:25 ON 01 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 17:14:34 ON 01 MAR 2004
L1               STRUCTURE UPLOADED
L2            86 S L1 SSS FULL

     FILE 'MARPAT' ENTERED AT 17:15:06 ON 01 MAR 2004
L3            45 S L1 SSS FULL

     FILE 'CAOLD' ENTERED AT 17:16:02 ON 01 MAR 2004
L4             0 S LL1 SSS FULL
                 S L1

     FILE 'REGISTRY' ENTERED AT 17:16:27 ON 01 MAR 2004
L5            86 S L1 SSS FULL

     FILE 'CAOLD' ENTERED AT 17:16:27 ON 01 MAR 2004
L6             1 S L5 SSS FULL

     FILE 'CAPLUS' ENTERED AT 17:16:39 ON 01 MAR 2004
L7            22 S L2
L8            45 S L3
L9          2306 S L 6
L10           22 S L6

=> d l7 fbib hitstr abs total

L7   ANSWER 1 OF 22  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:841743  CAPLUS
DN   140:93755
TI   A concise synthesis of ortho-substituted aryl-acrylamides-potent
     activators of soluble guanylyl cyclase
AU   Zhang, Henry Q.; Xia, Zhiren; Kolasa, Teodozyj; Dinges, Jurgen
CS   Global Pharmaceutical Research and Development, Department of Medicinal
     Chemistry Technologies (R-4CP), Abbott Laboratories, Abbott Park, IL,
     60064, USA
SO   Tetrahedron Letters (2003), 44(48), 8661-8663
     CODEN: TELEAY; ISSN: 0040-4039
PB   Elsevier Science B.V.
DT   Journal
LA   English
IT   643763-52-4P, 3-[2-(Phenylthio)phenyl]-2-propenoic acid
     643763-53-5P 643763-54-6P 643763-55-7P
     643763-56-8P 643763-57-9P 643763-58-0P
     643763-59-1P 643763-60-4P 643763-61-5P
     643763-62-6P 643763-63-7P 643763-64-8P
     643763-65-9P 643763-66-0P 643763-67-1P
     643763-68-2P 643763-69-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of N-[(dimethylamino)alkyl][(thio)phenyl]propenamides and their
```

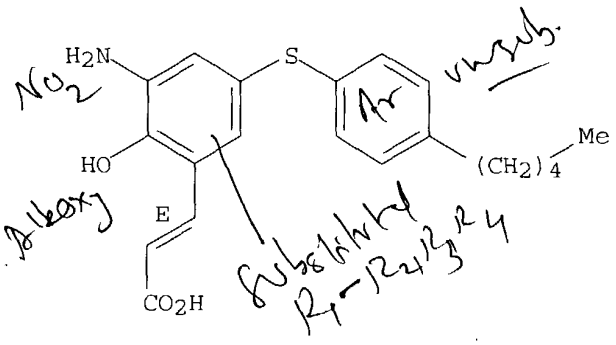
CO2R7; R7 = H, lower alkyl] or their pharmaceutically acceptable salts, useful as inhibitors of leukotriene biosynthesis (no data), are claimed. These compds. are useful as anti-asthmatic, anti-allergic, antiinflammatory, and cytoprotective agents (no data).

L10 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:504990 CAPLUS
DN 99:104990
TI 2-Aminophenol derivatives
IN Miyamoto, Tsumoru; Mohri, Tetsuya; Shimoji, Katsuichi; Wakatsuka, Hirohisa; Itoh, Hiroyuki; Hayashi, Masaki; Hashimoto, Shinsuke
PA Ono Pharmaceutical Co., Ltd. , Japan
SO Eur. Pat. Appl., 73 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

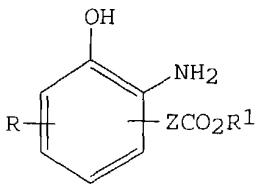
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 81321	A1	19830615	EP 1982-306277	19821125
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
			JP 1981-187730	19811125
JP 58090534	A2	19830530	JP 1981-187730	19811125

IT **86981-51-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 86981-51-3 CAPLUS
CN 2-Propenoic acid, 3-[3-amino-2-hydroxy-5-[(4-pentylphenyl)thio]phenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



GI

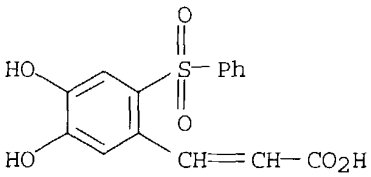


I

AB The title compds. (I; R = H, alkyl, alkoxy, halo, 4-R2C6H4S; R1 = H,

alkyl, 4-PhC6H4CH2; R2 = H, alkyl; Z = alkylene, alkenylene) were prepared Thus, (E)-3,2-R3(HO)C6H3CH:CHCO2R4 (II; R3 = R4 = H) was nitrated and esterified to give II (R3 = NO2, R4 = Et). This was reduced with NaSH to give II.HCl (R3 = NH2, R4 = Et) (III). At 0.5 μM and 1μM, resp., III gave 50% inhibition of 5-lipoxygenase and cyclooxygenase of guinea pig polymorphonuclear leukocytes.

L10 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:59590 CAPLUS
DN 98:59590
TI Use of thin-layer chromatography for determination of polyhydric phenols and quinones in wastewaters and reservoirs
AU Timofeeva, S. S.
CS Irkutsk. Gos. Univ., Irkutsk, USSR
SO Deposited Doc. (1981), VINITI 4990-81, 23 pp. Avail.: VINITI
DT Report
LA Russian
IT **58058-71-2**
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in water and wastewater, thin-layer chromatog. in)
RN 58058-71-2 CAPLUS
CN 2-Propenoic acid, 3-[4,5-dihydroxy-2-(phenylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



AB Monohydric and polyhydric phenols and their phenylsulfonyl derivs. were determined by thin-layer chromatog. with silica gel, Al2O3, and 2% HCl-treated Al2O3 as adsorbents. The use of spot area measurement on the chromatogram is recommended for the determination of small (≤20 μg) amts. The coeffs. of variation in determining the phenylsulfonyl derivs. of phenols by elution with subsequent spectrophotometry were 3-11%.

L10 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:479105 CAPLUS
DN 95:79105
TI Promotion of quinone formation from exogenous polyphenols in leaf homogenates of sunflower grown under conditions of a boron deficiency
AU Shkolnik, M. Ya.; Krupnikova, T. A.; Timofeeva, S. S.; Stom, D. I.
CS V. L. Komarov Bot. Inst., Leningrad, USSR
SO Fiziologiya Rastenii (Moscow) (1981), 28(3), 541-6
CODEN: FZRSAV; ISSN: 0015-3303
DT Journal
LA Russian
IT **58058-71-2**
RL: FORM (Formation, nonpreparative)
(formation of, in sunflower leaf homogenates from exogenous polyphenols, boron deficiency effect on)
RN 58058-71-2 CAPLUS
CN 2-Propenoic acid, 3-[4,5-dihydroxy-2-(phenylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)